SAND2020-3076PE

Nonlocal Models and Peridynamics

Computational Math Seminar
School of Mathematical and Statistical Sciences
Clemson University
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Michael Parks
Center for Computing Research
Sandia National Laboratories

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Outline

- ❑ **Local Models, Nonlocal Models, and Length Scales**
- ❑ **Peridynamics Overview**
- ❑ **Example Computations**
- ❑ **Material Models and Failure Models**
- ❑ **Discretizations and Numerical Methods**
- ❑ **Asymptotically Compatible Discretizations**
- ❑ **Nonlocal Calculus**
- ❑ **Condition Number Analysis**

Mathematical Models

- **We use numerical solutions of mathematical models to inform high-consequence decisions.**
- **When is a mathematical model any good?**
- **Model Validation**
  - "Am I solving the right problem?"
  - Is the model sufficient for the application?
  - Is model quantitatively predictive?
  - Is model predictive outside of its calibration range?
- **Model Verification**
  - "Am I solving the problem right?"
  - Are the equations solved correctly?
  - Can model produce known analytical solutions?

"All models are wrong, but some are useful."
- George Box

- **We are trained from an early age to use (local) PDE-based models to describe physical phenomena.**
- Today, I'll discuss physical phenomena for which classical models appear inadequate, and for which another mathematical approach may be required.
- Let's start with a discussion on local and nonlocal models, length scales, and multiscale models.

Local and Nonlocal Models

- **Local models** depend upon function values and derivatives at a point
  - $f_1(x) = u_{xx}(x)$, $f_2(x) = a\, u_{xx}(x) + b\, u_{xxxx}(x)$
- **Nonlocal models** depend upon values of a function at many points
  - $f_3(x) = \int_{-\delta}^{\delta} (u(x+y) - u(x))\, dy$
- **Some models possess length scales. How can we identify and control them?**
- Scale invariant (self-similar): $f_1(x) = u_{xx}(x)$
  - If x is rescaled, there exists a rescaling of u that preserves equation
- A single length scale: $f_2(x) = a\, u_{xx}(x) + b\, u_{xxxx}(x)$
  - Length scale is sqrt(b/a) (from dimensional analysis)
  - Rescaling x can make first term dominant or second term dominant
- An infinite number of length scales: $f_3(x) = \int_{-\delta}^{\delta} (u(x+y) - u(x))\, dy$
  - Consider a series expansion: $f_3(x) = \frac{\delta^3}{3} u_{xx}(x) + \frac{\delta^5}{60} u_{xxxx}(x) + \frac{\delta^7}{2520} u_{xxxxxx}(x) + \cdots$

At a fundamental level, multiscale modeling is about identification of length scales and control of model behavior at those length scales

Local and Nonlocal Models

- **We use PDE-based (local) models to describe most physical phenomena.**
  - Solid mechanics, fluid mechanics, electricity and magnetism, etc.

- **Classical PDE-based physics is descriptive of most (?) phenomena…**
  - **… except when it isn't.**

- **Classical models may cease to be descriptive if they cannot represent length scales of all dominant physical processes they are attempting to capture.**
  - This includes most ***multiscale*** phenomena (example: fracture, failure, etc.)

- **When our PDE-based models cease to be descriptive, our typical first response is to modify them (or modify their discretization) to make them to elicit desired behavior.**

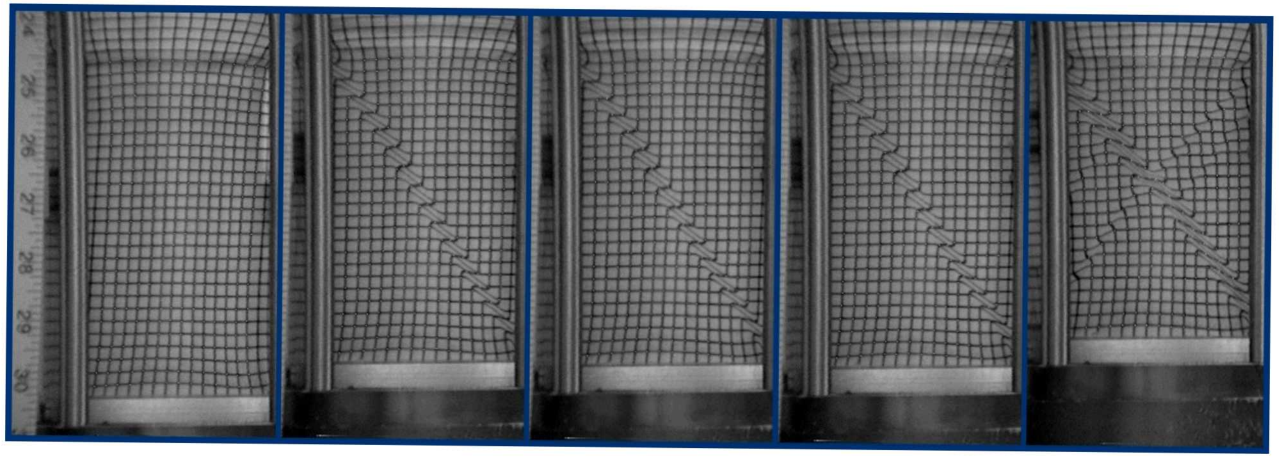
- **The critical issue at hand is representation and control of behavior at multiple length scales.**
- **In practice, nonlocal models do this fairly naturally.**

- **A first-principles matching of length scales in nonlocal models to length scales in observed physical phenomena remains an open question for many applications.**

Nonlocal Models & Length Scale Effects

- **Length scale effects arise in many applications**

Specimen before test



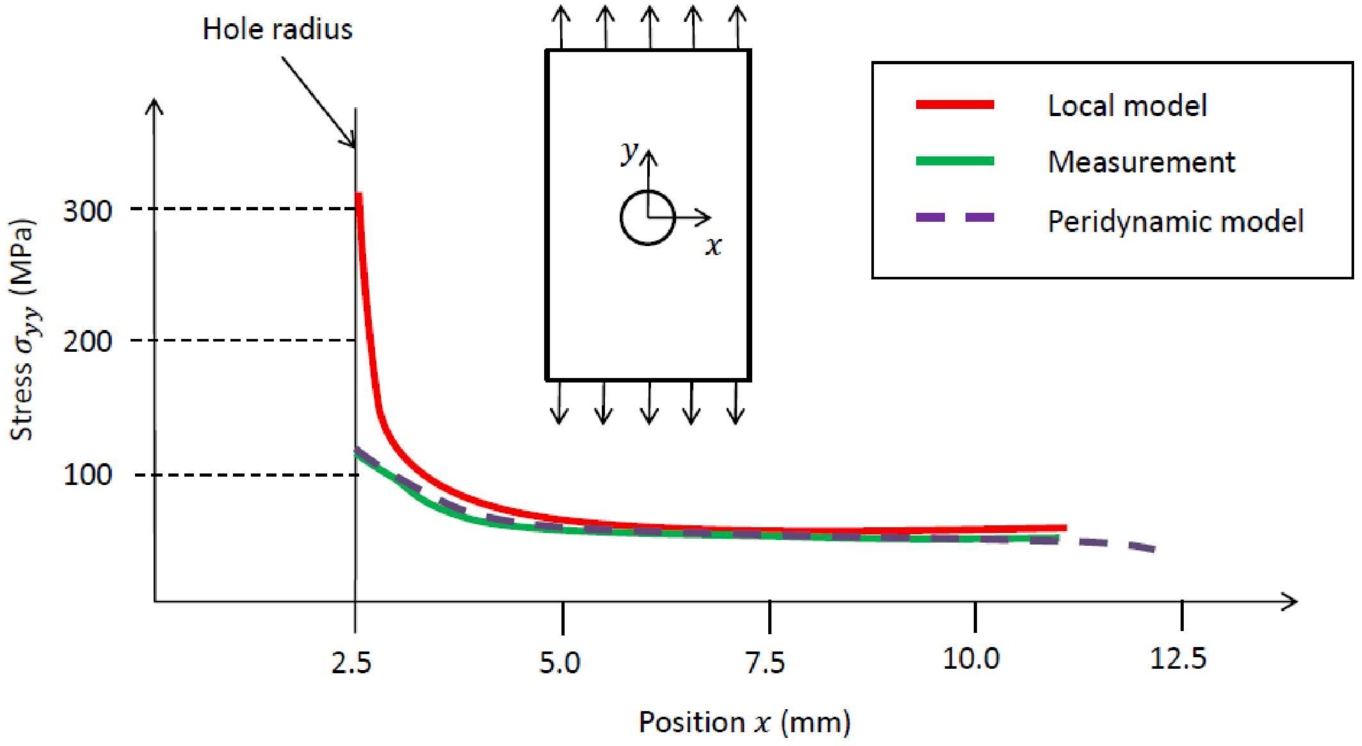
Onset of strain localization into shear band for F-75 Ottawa sand*

- **Example: Size of shear band (strain localization)**
- A shear band is a narrow zone of intense shearing that developing during severe deformation of ductile materials.
- Finite element models of shear bands show **size of band decrease as mesh is refined**, meaning mesh length scale is controlling shear band size (nonphysical)!
- Higher gradient models introduced to control this behavior. Introduces additional length scales (ad-hoc).
- Nonlocal models can preserve size of shear band under mesh refinement.

* http://web.utk.edu/~alshibli/research/MGM/F75-Ottawa.php

Nonlocal Models & Length Scale Effects

- **Length scale effects arise in many applications**

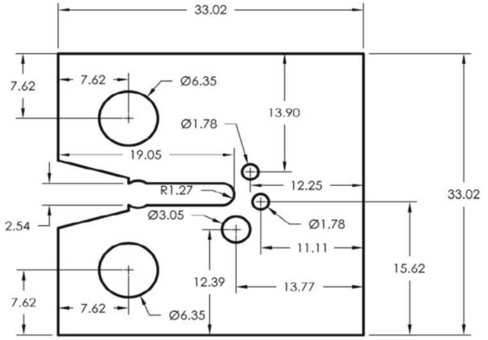


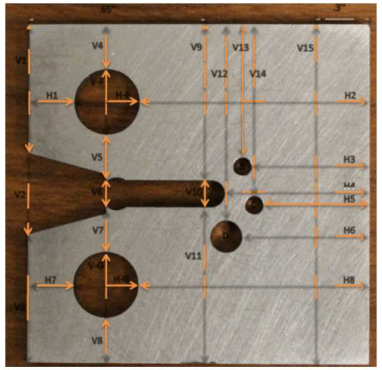
- **Heterogeneous media***
  - Comparison of stress along the midplane in an open hole tension test on a fabric-reinforced composite.
  - Local theory over-predicts the stress concentration, as compared with optically measured data.
  - Peridynamic model has better agreement, apparently due to nonlocality.

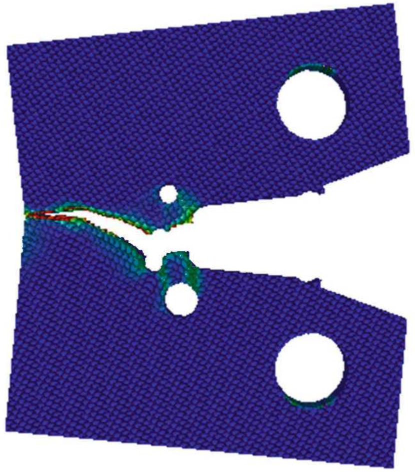
*S.A. Silling, *Origin and Effect of Nonlocality in a Composite*, Sandia Technical Report SAND2013-8140, 2013.

Nonlocal Models & Length Scale Effects

- ❑ **Length scale effects arise in many applications**







- ❑ **Fracture and Failure***
- ❑ Classical theory predicts infinite stress (1/sqrt(r) singularity) at crack tip.
- ❑ Classical theory (based on PDEs) not defined on crack surfaces
- ❑ Common numerical approaches (XFEM, etc.) enrich solution space with (for example) heaviside functions to allow admission of discontinuous solutions
- ❑ Nonlocal models avoid infinities and are defined everywhere (on and off cracks).

*B. Boyce, et al, The Sandia Fracture Challenge: Blind Round Robin Predictions of Ductile Tearing, Int J Fract. 186:5–68, 2014.

Nonlocal Models

- **Nonlocality and nonlocal models are not a new concept.**

- There are a large number of nonlocal models used in computational science
  - Particle models: DPD, SPH, MPM, MD, …
  - Nonlocal continuum models: Eringen, Bazant, Kunin, Kromer, …

- Peridynamics, a nonlocal extension of classical continuum mechanics, has been demonstrated to be a superset of some prior nonlocal models:
  - SPH [G.C. Ganzenmüller, S. Hiermaier, M. May, 2015]
  - MD [Seleson, P, Gunzburger, Lehoucq, 2009]
  - Theories of Kunin [Kunin, 1982]
  - Theories of Rogula [Rogula, 1982]

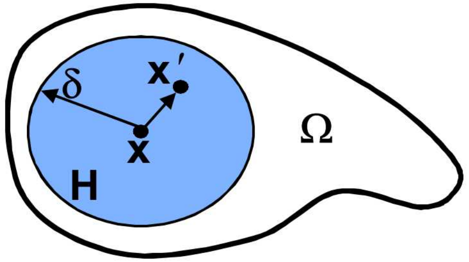
Peridynamics Overview

What is Peridynamics?

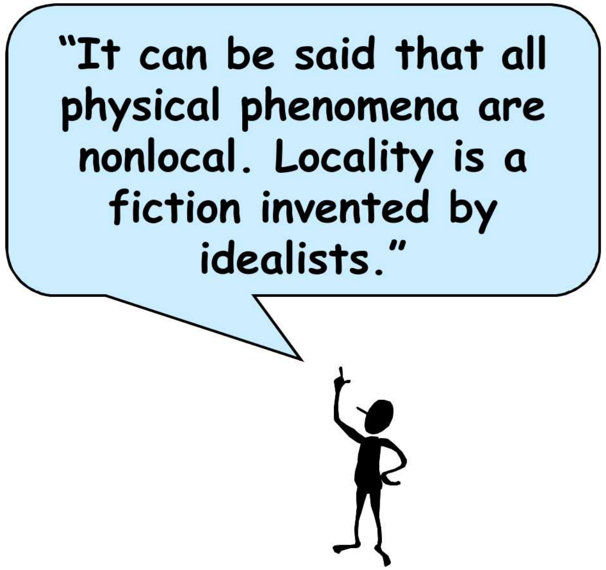
- ❑ **Peridynamics is a nonlocal extension of classical solid mechanics**
- ❑ **Peridynamic equation of motion (integral, nonlocal)**

$$\rho\ddot{u}(x,t) = \int_{H_x} f(u(x') - u(x), x'-x)dV' + b(x,t)$$

  - ❑ Replace PDEs with integral equations
  - ❑ Utilize same equation everywhere; nothing "special" about cracks
  - ❑ No assumption of differentiable fields (admits fracture)
  - ❑ No obstacle to integrating nonsmooth functions
  - ❑ $f(\cdot, \cdot)$ is "force" function; contains constitutive model
  - ❑ f = 0 for points x,x' more than δ apart (like cutoff radius in MD!)
  - ❑ Peridynamics is "continuum form of molecular dynamics"
- ❑ **Impact**
  - ❑ Nonlocality
  - ❑ Larger solution space (fracture)
  - ❑ Account for material behavior at small & large length scales (multiscale material model)
- ❑ **Ancestors**
  - ❑ Kröner, Eringen, Edelen, Kunin, Rogula, etc.



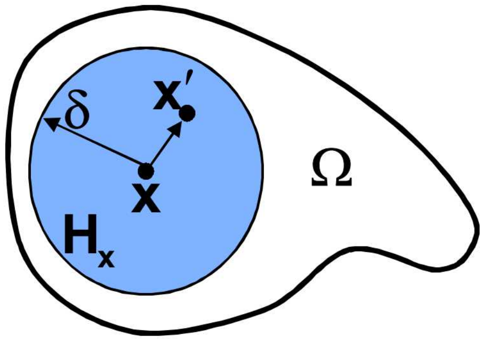
Point x interacts directly with all points x' within H



A. Cemal Eringen

Peridynamics: The Basics

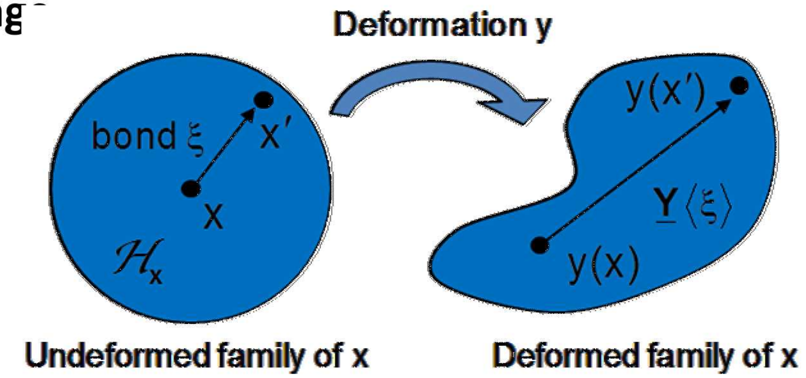
- **Horizon and family**
  - **Point x interacts directly with all points with distance δ (horizon)**
  - **Material within distance δ of x is denoted H_x (family of x)**



- **Bonds and bond forces**
  - **Vector between x and any point in its family is called a bond: ξ = x' – x**
  - **Each bond has pairwise force density vector applied at both points: f(x', x, t)**
  - **This vector is determined jointly by collective deformation of H_x and collective deformation of $H_{x'}$**
  - **Bond forces are antisymmetric: f(x', x, t) = - f(x, x', t)**
  - **Bond degrade and fail, admitting damage, failure, and fracture**

- **Deformation state**
  - **Deformation state operator $\underline{Y}$ maps each bond ξ into its deformed imag**

$$\underline{\mathbf{Y}}\langle\xi\rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$$



Peridynamics: The Basics

- **Bonds and states**
  - **f(x′, x) has contributions from material models at both x and x′**

$$\mathbf{f}(\mathbf{x}',\mathbf{x}) = \underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}',t]\langle \mathbf{x}-\mathbf{x}'\rangle$$

  - **T[x] is the force state – it maps bonds onto bond force densities**
  - **T[x] is determined by the constitutive model $\underline{T} = \hat{\underline{T}}(\underline{Y})$, where $\hat{T}$ maps deformation state to force state**

- **Peridynamics vs. standard equations**

Relation	Peridynamic theory	Standard theory
Kinematics	$\underline{\mathbf{Y}}\langle \mathbf{x}'-\mathbf{x}\rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear momentum balance	$\rho\ddot{\mathbf{u}}(\mathbf{x}) = \int_{H_x} \left(\underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}']\langle \mathbf{x}-\mathbf{x}'\rangle\right) dV_{x'} + \mathbf{b}(\mathbf{x})$	$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \nabla\cdot\sigma(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive model	$\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$	$\sigma = \hat{\sigma}(\mathbf{F})$
Angular momentum balance	$\int_{H_x} \underline{\mathbf{Y}}\langle \mathbf{x}'-\mathbf{x}\rangle \times \underline{\mathbf{T}}\langle \mathbf{x}'-\mathbf{x}\rangle dV_{x'} = 0$	$\sigma = \sigma^T$
Elasticity	$\underline{\mathbf{T}} = W_{\underline{Y}}$ (Frechet derivative)	$\sigma = W_F$ (tensor gradient)
First law of thermodynamics	$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + h + r$	$\dot{\varepsilon} = \sigma\cdot\dot{\mathbf{F}} + h + r$

Peridynamics: The Basics

❑ Mechanical Properties of Peridynamics

- ❑ Conserves energy (in absence of fracture, plastic deformation, etc.)
- ❑ Conserves linear & angular momentum (always)
- ❑ Obeys the laws of thermodynamics (restrictions on constitutive models)

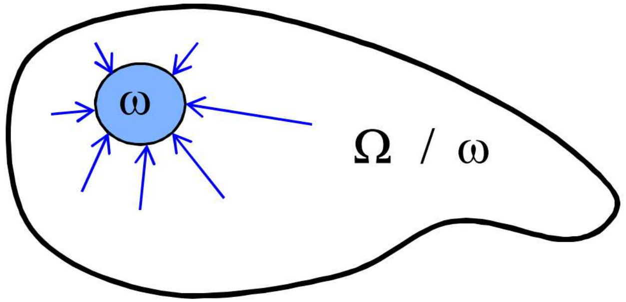
❑ Example: Conservation of Momentum

- ❑ Rate of change of momentum of material within ω equals force of body outside ω acting upon ω plus external body force upon ω:

$$\frac{d}{dt}\int_{\omega} \rho \dot{u}(x,t) dV_x = \int_{\omega}\int_{\Omega/\omega} \left(T[x,t]\langle x' - x \rangle - T[x',t]\langle x - x' \rangle \right) dV_{x'} dV_x + \int_{\omega} b(x,t) dV_x$$

- ❑ No self-interaction

$$\int_{\omega}\int_{\omega} \left(T[x,t]\langle x' - x \rangle - T[x',t]\langle x - x' \rangle \right) dV_{x'} dV_x = 0$$



Peridynamics: The Basics

Energy Balance

- **T is work conjugate to Y:**
- **This leads to energy balance (first law of thermodynamics)**

$$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} + \mathbf{q} + \mathbf{r}$$

Peridynamic equivalent of stress power $\sigma \cdot \dot{\mathbf{F}}$

where

- ε **= internal energy density**
- **q = rate of heat transport**
- **r = energy source rate**

Thermodynamic Admissibility for Constitutive Models

- **Second law of thermodynamics (Clausius-Duhem inequality):**

$$\theta\dot{\eta} \geq \mathbf{q} + \mathbf{r}$$

where

- θ **= absolute temperature**
- η **= entropy density**
- **Combining with first law gives thermodynamic admissibility condition for constitutive models:**

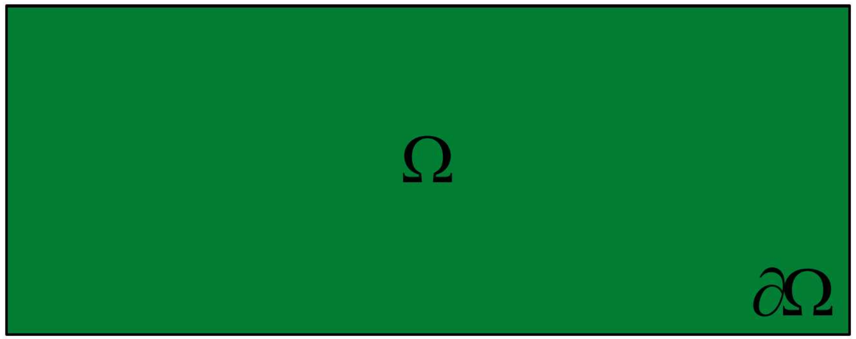
$$\underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} - \dot{\theta}\eta - \dot{\psi} \geq \mathbf{0}$$

where

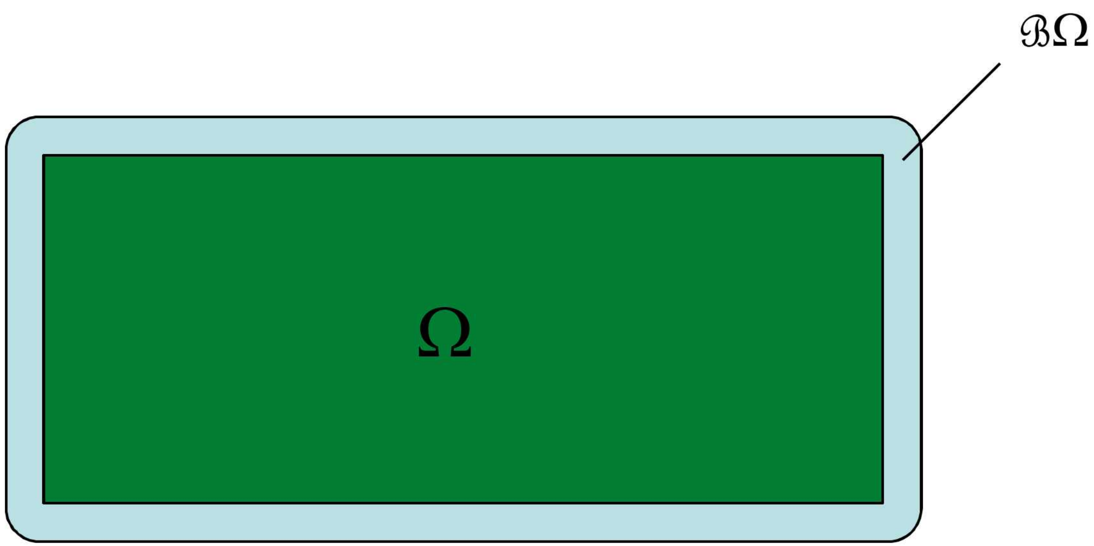
- $\psi = \varepsilon - \theta\eta$ **is free energy density**

Nonlocal Boundary Conditions

- For local models (for example, PDE-based models), we apply boundary conditions on the boundary of the domain (hence the name)



- A Peridynamic "boundary" becomes a volumetric region, sometimes called a "nonlocal boundary", "collar", etc.
- Boundary conditions for these models are called "nonlocal boundary conditions", "volume constraints", etc.



Example Computations

Codes

- ❑ **PDLAMMPS (Peridynamics-in-LAMMPS) (Open source, C++)**
  - ❑ **Developers: Parks, Seleson, Plimpton, Silling, Lehoucq**
  - ❑ **Particular discretization of PD has computational structure of molecular dynamics (MD)**
  - ❑ **LAMMPS: Sandia's open-source massively parallel MD code (lammps.sandia.gov)**
  - ❑ **More info & user guide: www.sandia.gov/~mlparks**

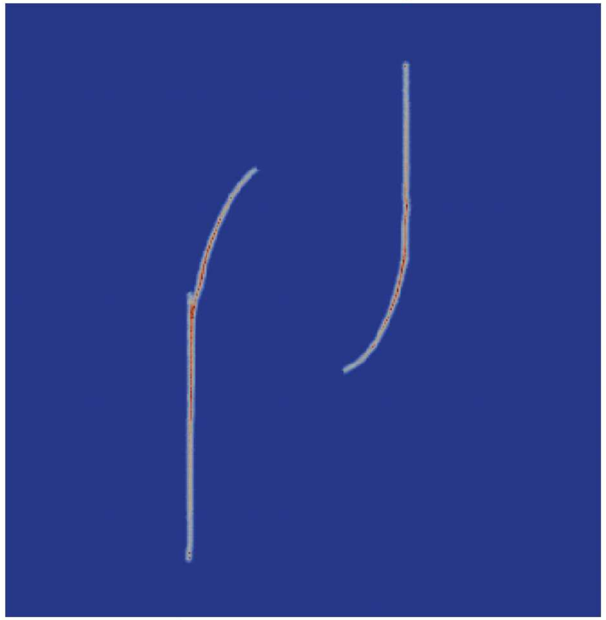
- ❑ **Peridigm (Open Source, C++)**
  - ❑ **http://peridigm.sandia.gov; http://github.com/peridigm/peridigm**
  - ❑ **Developers: Parks, Littlewood, Mitchell, Silling**
  - ❑ **Intended as Sandia's primary open-source PD code**
  - ❑ **Built upon Sandia's Trilinos Project (trilinos.sandia.gov)**
  - ❑ **Massively parallel**
  - ❑ **Explicit, implicit time integration**
  - ❑ **State-based linear elastic, elastic-plasticity, viscoelastic models**
  - ❑ **DAKOTA interface for UQ/optimization/calibration, etc. (dakota.sandia.gov)**

Two Interacting Cracks

- **Offset notches thin rectangular elastic plate**
  - **Uniaxial strain applied from sides**
  - **Approaching cracks produce "en passant" crack pattern**

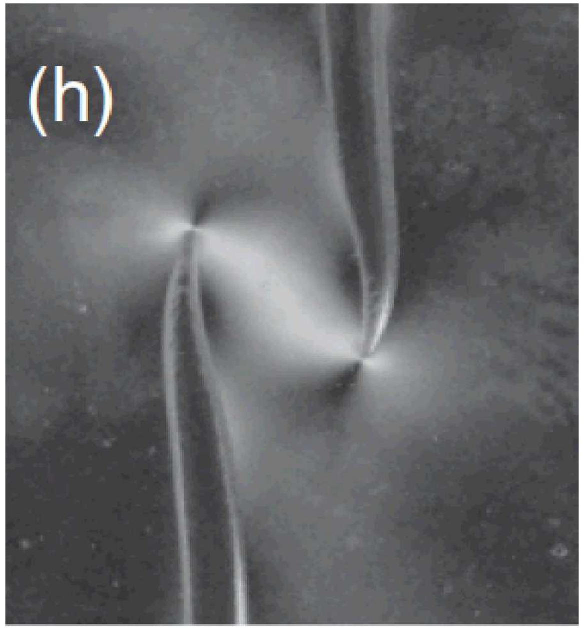
Simulation performed with PDLAMMPS

Pre-notch



Pre-notch

Peridynamics



Physical Experiment*

* M. Fender, F. Lechenault, and K. Daniels, Universal Shapes Formed by Two Interacting Cracks, Phys. Rev. Lett. 105, 125505 (2010) .

Fracture in Glass Plate

- Dynamic brittle fracture in glass
  - Joint with Florin Bobaru, Youn-Doh Ha, & Stewart Silling

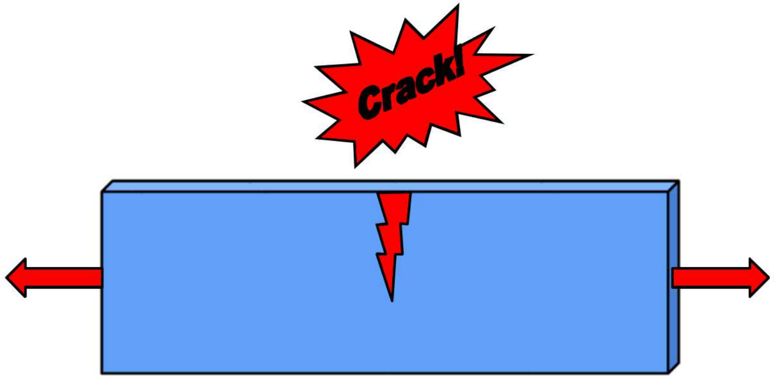
Simulation performed with PDLAMMPS

- Soda-lime glass plate (microscope slide)
  - Dimensions: 3” x 1” x 0.05”
  - Density: 2.44 g/cm3
  - Elastic Modulus: 79.0 Gpa

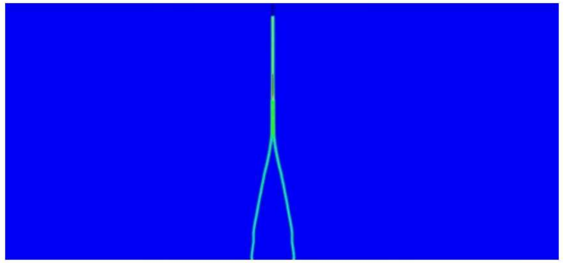
- Discretization (finest)
  - Mesh spacing: 35 microns
  - Approx. 82 million particles
  - Time: 50 microseconds (20k timesteps)

Setup

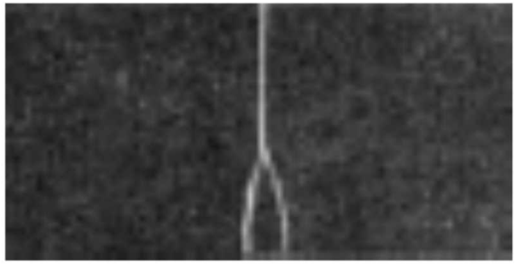
- Glass microscope slide
- Dimensions: 3” x 1” x 0.05”
- Notch at top, pull on ends



Results



Peridynamics



Physical Experiment*

Strain Energy Density

*S F. Bowden, J. Brunton, J. Field, and A. Heyes, *Controlled fracture of brittle solids and interruption of electrical current*, Nature, 216, 42, pp.38-42, 1967.

Fracture in Glass Plate

- **Dawn (LLNL): IBM BG/P System**
  - 500 teraflops; 147,456 cores
- **Part of Sequoia procurement**
  - 20 petaflops; 1.6 million cores
- **Discretization (finest)**
  - Mesh spacing: 35 microns
  - Approx. 82 million particles
  - Time: 50 microseconds (20k timesteps)
  - 6 hours on 65k cores
- **Largest peridynamic simulations in history**

Simulation performed with PDLAMMPS

Dawn **at LLNL**

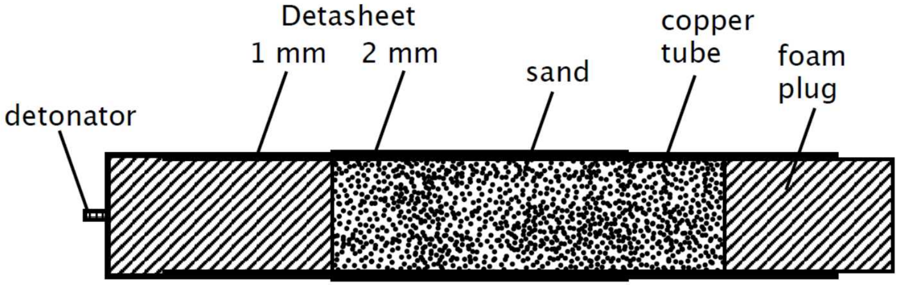
Weak Scaling Results

# Cores	# Particles	Particles/Core	Runtime (sec)	T(P)/T(P=512)
512	262,144	4096	14.417	1.000
4,096	2,097,152	4096	14.708	0.980
32,768	16,777,216	4096	15.275	0.963

Explosively Compressed Cylinder*

- Motived by experiments of Vogler & Lappo*
- Commonly used for consolidation of powders
- Copper cylinders filled with granular material and wrapped with Detasheet explosive
- Polyurethane foam plugs used to keep granular sample in tube.

- Geometry and Material Properties
  - Copper tubes 305 mm long, ID 50.8 mm, wall thickness of 1.52 mm
  - PETN based Detasheet with thicknesses of 1, 2, 4, or 6 mm were used, and a
  - Detonation traveled down length of tube, compressing both tube and sand fill



Cylinder schematic

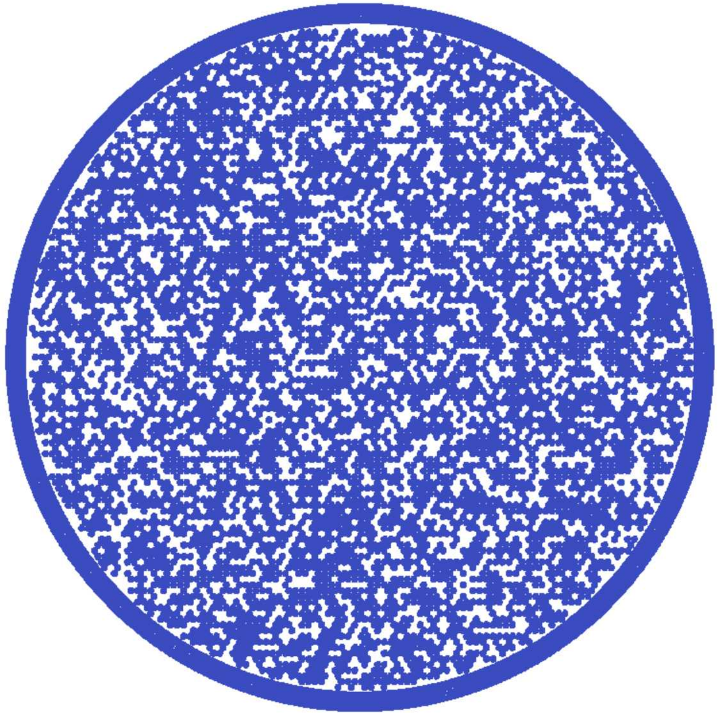
Cylinder after compression

* T.J. Vogler and K.M. Lappo, Cylindrical Compaction of Granular Ceramics: Experiments and Simulations, The 12th Hypervelocity Impact Symposium. 2012.

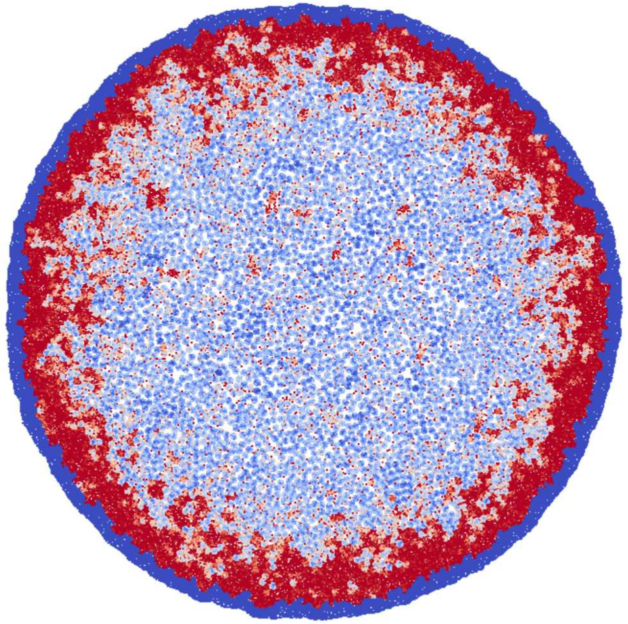
Explosively Compressed Cylinder

- ❑ **Peridigm computational results (with C. Hoffarth, D. Littlewood)**
- ❑ **Color indicates damage (blue = undamaged, red = damaged)**

Simulation performed with Peridigm



Before



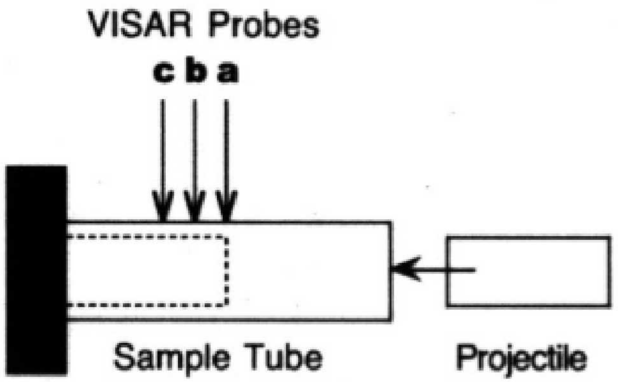
After

Expanding Tube Simulation**

- **Experimental Setup**
  - **Tube expansion via collision of Lexan projectile and plug within AerMet tube**
  - **Accurate recording of velocity and displacement on tube surface**

- **Modeling Approach**
  - **AerMet tube modeled with peridynamics, elastic-plastic material model with linear hardening**
  - **Lexan plugs modeled with classical FEM, equation-of-state Johnson-Cook material model**
  - **Interaction via contact algorithm**

Simulation performed with Sierra/SolidMechanics



Experimental setup*

Model discretization

Vogler, T.J., Thornhill, T.F., Reinhart, W.D., Chhabidas, L.C., Grady, D.E., Wilson, L.T., Hurricane, O.A., and Sunwoo, A. Fragmentation of materials in expanding tube experiments. *International Journal of Impact Engineering*, 29:735-746, 2003.

** D. Littlewood. 2010. Simulation of dynamic fracture using peridynamics, finite element modeling, and contact. Proceedings of the ASME 2010 International Mechanical Engineering Congress and Exposition, British Columbia, Canada.

Expanding Tube Simulation**

Simulation performed with Sierra/SolidMechanics

AerMet Tube

- Peridynamics
- Elastic-plastic constitutive model
- 73,676 sphere elements
- Horizon set to five times element radius

Parameter	Value
Density	7.87 g/cm^3
Young's Modulus	194.4 GPa
Poisson's Ratio	0.3
Yield Stress	1.72 GPa
Hardening Modulus	1.94 GPa
Critical Stretch	0.02

Lexan Projectile/Plug

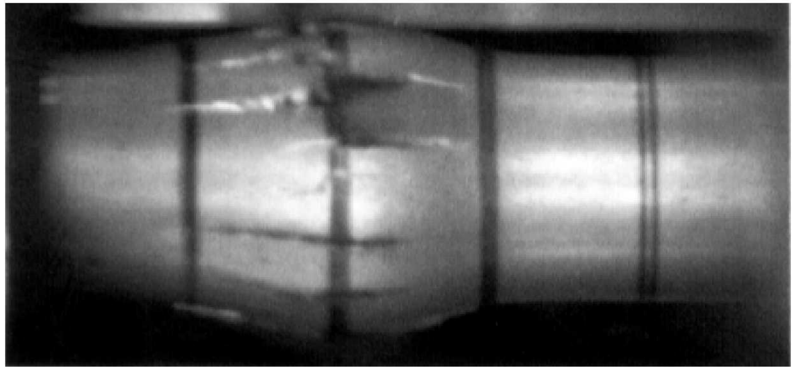
- Classical FEM
- Johnson-Cook constitutive model
- 53,214 hexahedron elements

Parameter	Value
Density	1.19 g/cm^3
Young's Modulus	2.54 GPa
Poisson's Ratio	0.344
Yield Stress	75.8 MPa
Hardening Constant *B*	68.9 MPa
Rate Constant C	0.0
Hardening Exponent *N*	1.0
Thermal Exponent *M*	1.85
Reference Temperature	70.0 ° F
Melting Temperature	500.0 ° F

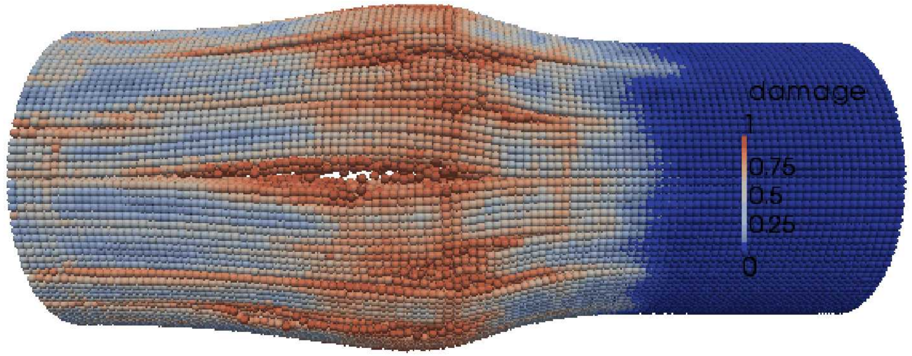
** D. Littlewood. 2010. Simulation of dynamic fracture using peridynamics, finite element modeling, and contact. Proceedings of the ASME 2010 International Mechanical Engineering Congress and Exposition, British Columbia, Canada.

Expanding Tube Simulation**

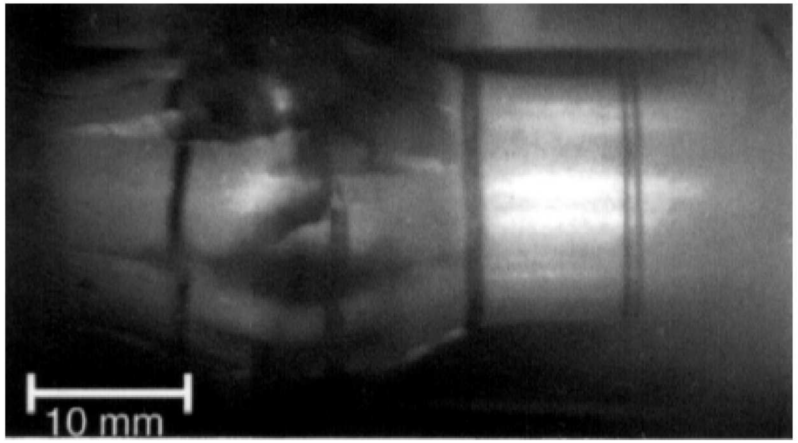
Simulation performed with Sierra/SolidMechanics



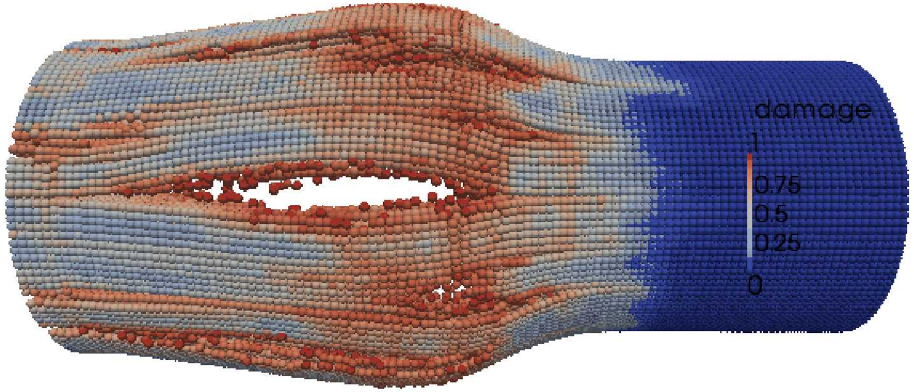
Experimental image at 15.4 microseconds*



Simulation at 15.4 microseconds**



Experimental image at 23.4 microseconds*



Simulation at 23.4 microseconds**

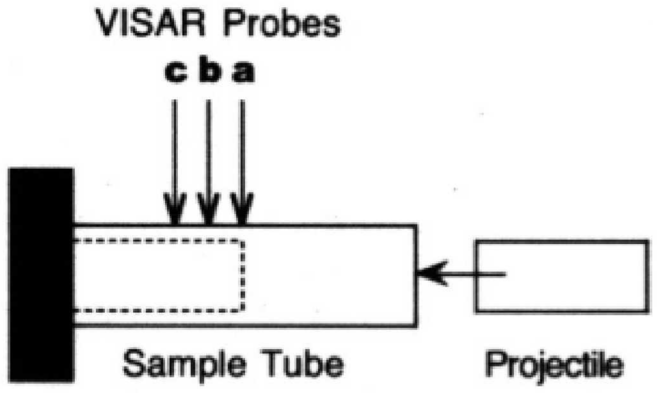
Vogler, T.J., Thornhill, T.F., Reinhart, W.D., Chhabidas, L.C., Grady, D.E., Wilson, L.T., Hurricane, O.A., and Sunwoo, A. Fragmentation of materials in expanding tube experiments. *International Journal of Impact Engineering*, 29:735-746, 2003.

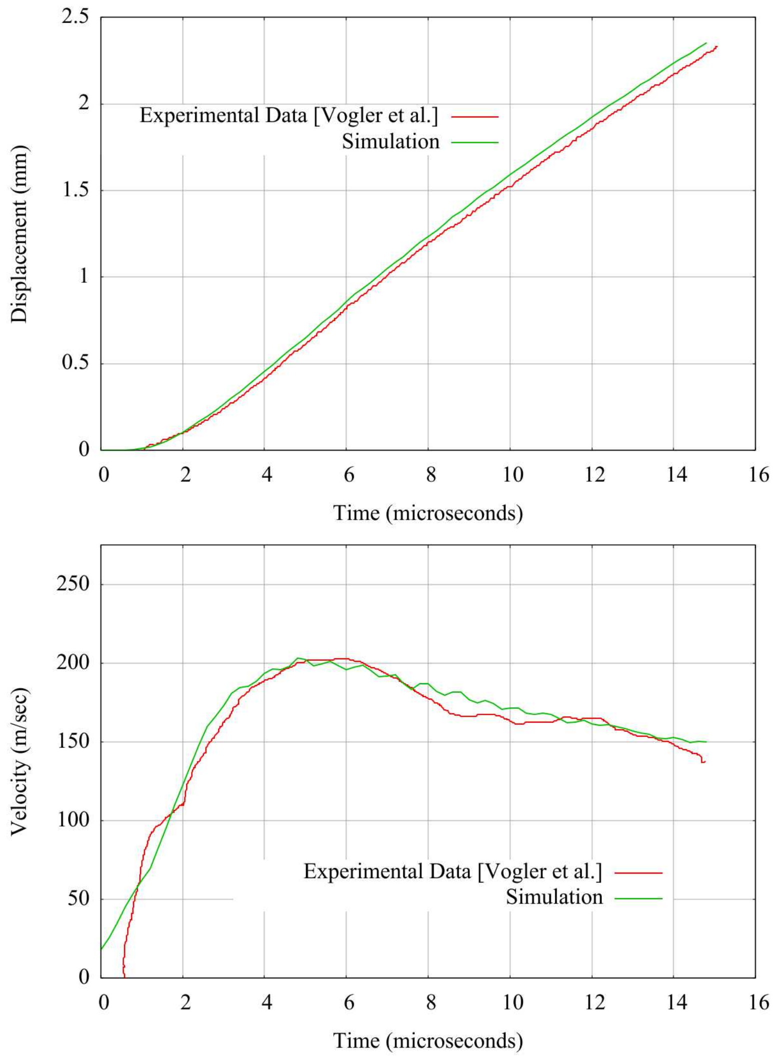
** D. Littlewood. 2010. Simulation of dynamic fracture using peridynamics, finite element modeling, and contact. Proceedings of the ASME 2010 International Mechanical Engineering Congress and Exposition, British Columbia, Canada.

Expanding Tube Simulation**

Simulation performed with Sierra/SolidMechanics

Displacement and velocity on tube surface at probe position A





Vogler, T.J., Thornhill, T.F., Reinhart, W.D., Chhabidas, L.C., Grady, D.E., Wilson, L.T., Hurricane, O.A., and Sunwoo, A. Fragmentation of materials in expanding tube experiments. *International Journal of Impact Engineering*, 29:735-746, 2003.

** D. Littlewood. 2010. Simulation of dynamic fracture using peridynamics, finite element modeling, and contact. Proceedings of the ASME 2010 International Mechanical Engineering Congress and Exposition, British Columbia, Canada.

Material Models and Fracture Models

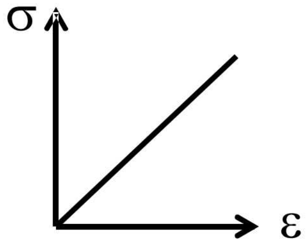
Peridynamic Material Models

- Quick survey of some material classes

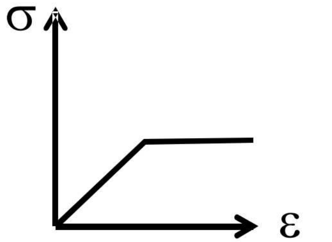
- **Linear Isotropic Elastic Materials**
  - Hooke's law
  - Returns to reference configuration when released
  - Example: spring

- **Elastic-Plastic Materials**
  - Elastic for small deformations (< 1% strain)
  - Deforms plastically for larger deformations
  - Example: spring (when stretched too far)

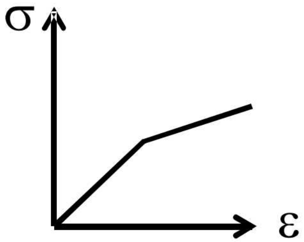
- **Viscoelastic Materials**
  - Exhibit viscous and elastic properties under deformation
  - Hysteresis in stress/strain curves
  - Example: skin (pinch it and let it recover)*



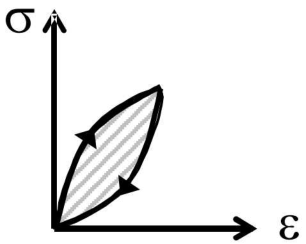
Linear Elastic



Elastic Perfectly Plastic



Elastic-Plastic (Strain Hardening)



Elastic Perfectly Plastic

- Can wrap classical material models (existing material libraries) in peridynamic "skin"
- PD codes (Peridigm, PDLAMMPS) allow users to define their own material models

* The longer it is pinched, the longer it takes to recover. Skin is also an *aging material* – young skin recovers more rapidly than old skin.

Peridynamic Material Modeling

- **Linear Peridynamic Solid (LPS)***
  - **Nonlocal analog to linear isotropic elastic solid**
  - **k is bulk modulus, μ is shear modulus**

$$\rho \ddot{\mathbf{u}}(\mathbf{x},t) = \int_{H} \left(\underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x} \rangle - \underline{\mathbf{T}}[\mathbf{x}',t]\langle \mathbf{x} - \mathbf{x}' \rangle \right) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

$$\underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x} \rangle = \left(\frac{3k\theta}{m} \underline{\omega}\,\underline{\mathbf{x}} + \frac{15\mu}{m} \underline{\omega}\,\mathbf{e}^{d} \right) \frac{\mathbf{x}' - \mathbf{x}}{\lVert \mathbf{x}' - \mathbf{x} \rVert}$$

*S.A. Silling, M. Epton, O. Weckner, J. Xu, & E. Askari, Peridynamic States and Constitutive Modeling, J. Elasticity, 88, pp. 151-184, 2007.

Peridynamic Material Models

- Elastic-Plastic Model*
  - Nonlocal analogue to perfect plasticity model
  - Relevant for ductile materials and ductile failure

- Rate equations and constraints
  - Additive decomposition of extension state: $e^d = e^{de} + e^{dp}$
  - Elastic force state relations:

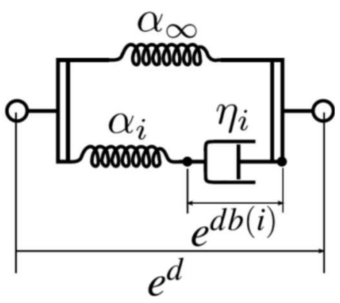
$$\mathbf{T}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x} \rangle = \left(\frac{3k\theta}{m} \underline{\omega}\underline{\mathbf{x}} + \alpha\underline{\omega}\left(e^d - e^{dP}\right) \right) \frac{\mathbf{y}' - \mathbf{y}}{\|\mathbf{y}' - \mathbf{y}\|}$$

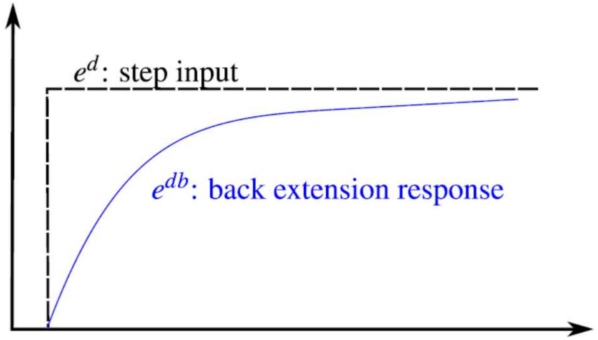
  - Elastic force state domain defined by yield surface/function that depends upon deviatoric force state:
    - $f(t_d) = \psi(t^d) - \psi_0 \leq 0$, where $\psi(t^d) = ½\|td\|^2$
  - Flow rule describing rate of plastic deformation: $\dot{e}^{dp} = \lambda \nabla^d \Psi$
  - Loading/un-loading conditions (Kuhn-Tucker constraints):
    - $\lambda > 0$, $f(t^d) \leq 0$,
    - Consistency condition: $\lambda \dot{f}(t^d) = 0$

* J. Mitchell, A Nonlocal, Ordinary, State-Based Plasticity Model for Peridynamics, SAND2011-3166, 2011.

Peridynamic Material Models

- **Viscoelastic Model***
  - **Nonlocal analog to standard linear solid**
  - **Applicable where rate effects important**
  - **Adds viscous terms to deviatoric portion of extension state; bulk response remains elastic**
  - **Logical intermediate step between fluid and solid**
  - **viscous fluid: little or no elastic resistance to shear (fluids flow) but resists compressive volumetric deformations**
  - **elastic solid: elastic resistance to both shear and volumetric deformations**





- **Viscoelastic Model***
  - **Nonlocal analog to standard linear solid**
  - **Scalar deviatoric force:** $\mathbf{t^d} = \eta_i \dot{\mathbf{e}}^{\mathbf{db}}$

$$= \alpha_i (\mathbf{e^d} - \mathbf{e^{db}})$$

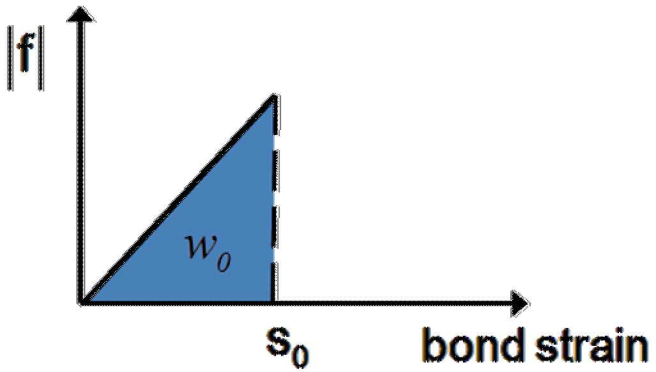
  - **Evolution equation:** $\dot{\mathbf{e}}^{\mathbf{db}} = \frac{1}{\tau^b}(\mathbf{e^d} - \mathbf{e^{db}})$

Memory Foam

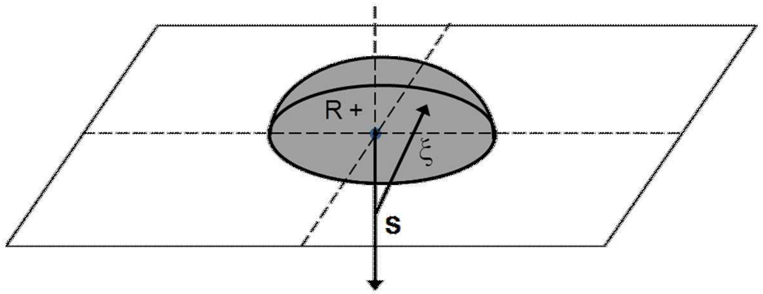
*J. Mitchell, A Non-local, Ordinary-State-Based Viscoelasticity Model for Peridynamics, SAND2011-8064, 2011.

Peridynamic Fracture Modeling

- **Fracture**
  - **Break bond if bond stretch s exceeds critical stretch s***
  - **If work to break bond ξ is $w_0(\xi)$, then energy release rate found by summing this work per unit crack area**

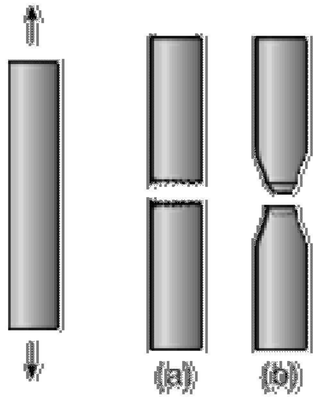


$$G = \int_0^{\delta} \int_{R_+} w_0(\xi) dV_\xi ds$$



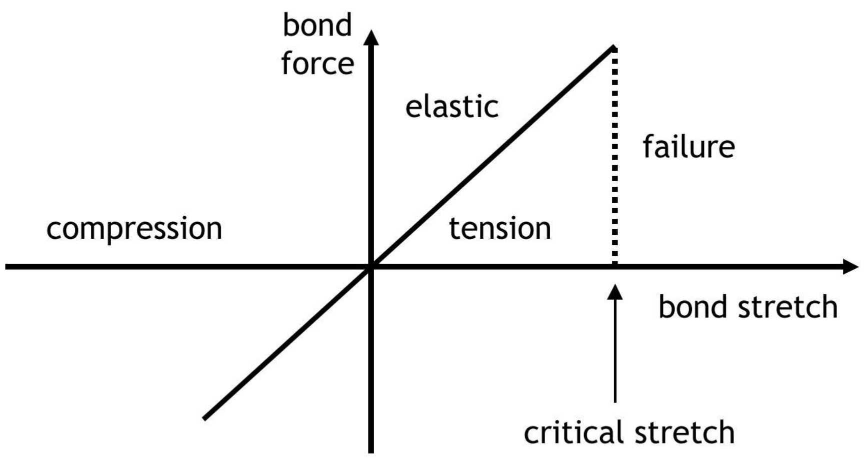
  - **Can then get the critical strain s* for bond breakage in terms of G (strain energy release rate), an experimentally measurable quantity**

- **Fracture**
  - **(a) Brittle**
  - **(b) Ductile**

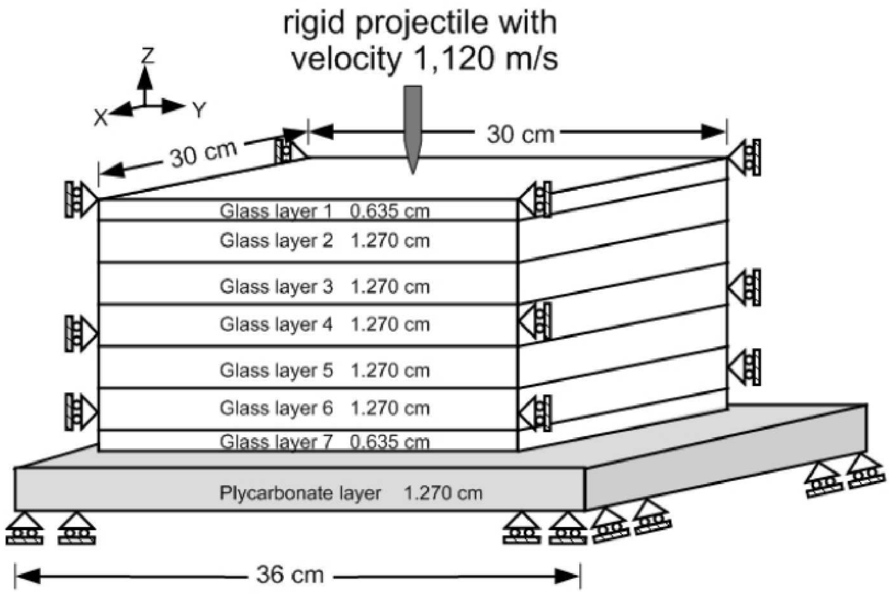


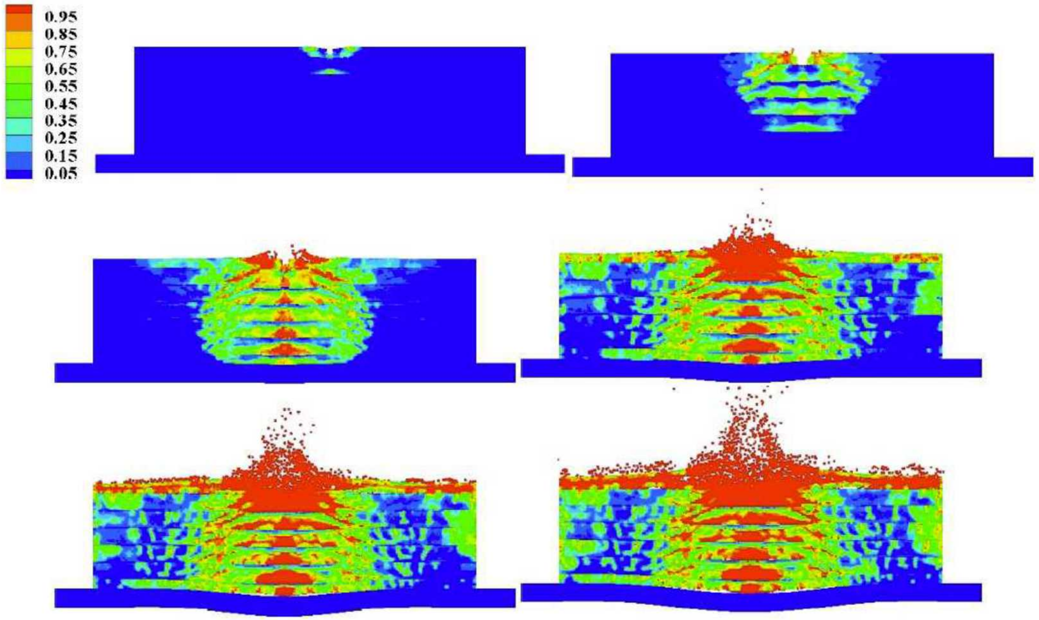
Peridynamic Fracture Modeling (Brittle)

- **Brittle Fracture**
  - **No plastic deformation takes place before failure**
  - **Typically involves catastrophic failure**
  - **Bond responds elastically until failure at critical stretch**



- **Example: Impact in Layered Glass**
  - **No plastic deformation takes place before failure**

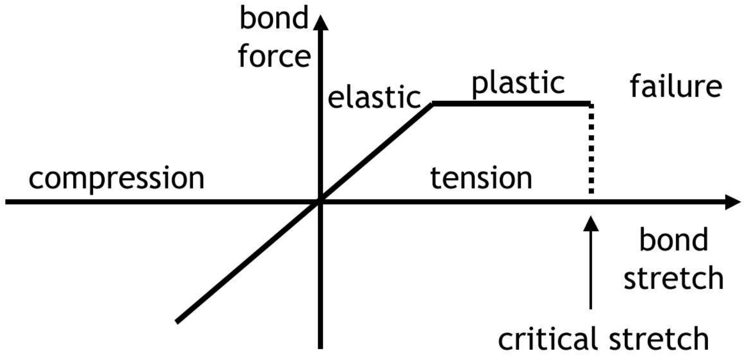




F. Bobaru, YD. Ha, and W. Hu, "Damage progression from impact in layered glass modeled with peridynamics", Open Engineering, 2(4): 551-561 (2012).

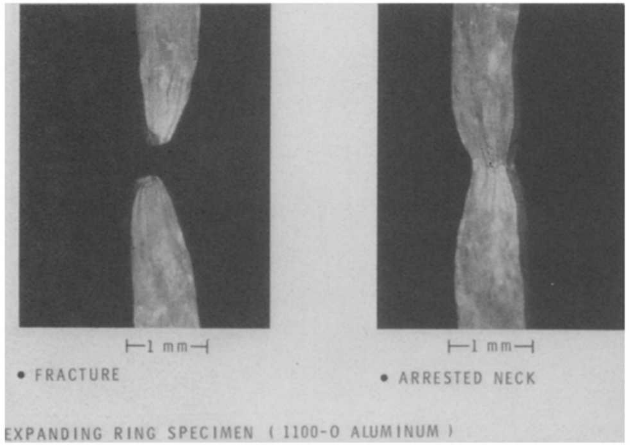
Peridynamic Fracture Modeling (Ductile)

- **Ductile fracture**
  - **Plastic deformation before failure**
  - **Can typically sustain large strain before failure**

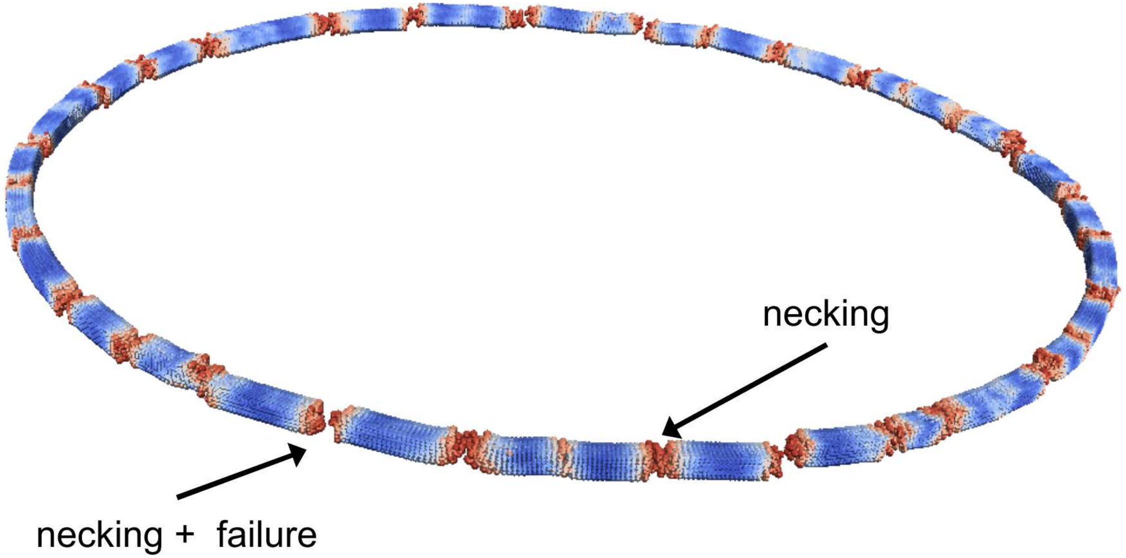


Simulation performed with Peridigm

- **Example: Electromagnetically loaded ring**
  - **1100-0 aluminum ring (ductile)**
  - **Motivated by ring fragmentation experiments of Grady & Benson***
  - **Used peridynamic elastic/plastic model****



Fracture and arrested neck region from dynamic expansion of ring*



* D. Grady, D. Benson, Fragmentation of metal rings by electromagnetic loading, Experimental Mechanics, 23(4), pp. 393-400, 1983

** J. Mitchell, A Nonlocal, Ordinary, State-Based Plasticity Model for Peridynamics, SAND2011-3166, 2011.

Discretizations and Numerical Methods

Discretizing Peridynamics

- **Peridynamics is a continuum model – You choose the discretization scheme**

- **Temporal discretization**
  - **Explicit time integration (Velocity-Verlet)**
  - **Implicit time integration (Newmark-beta method)**

- **Spatial discretization (weak form)**
  - **Nonlocal Galerkin finite elements**
  - **Nonlocal discontinuous Galerkin finite elements**

- **Spatial discretization (strong form)** ← Primary discretization used in production codes.
  - **Midpoint quadrature**
  - **Gauss quadrature***

- **Solvers**
  - **Nonlocal domain decomposition methods**
  - **Nonlocal multigrid**
  - **Nonlinear (Newton/Krylov, nonlinear CG)**
  - **Linear (preconditioned Krylov subspace methods)**

*E. Emmrich and O. Weckner, *The peridynamic equation and its spatial discretization, Math. Model. Anal.,* 12(1), pp. 17-27, 2007.

Nonlocal Weak Form

- **Prototype operator**

$$L\{u\}(x) = -\int_{\overline{\overline{\Omega}}} C(x,x')\left[u(x') - u(x)\right]dx'$$

$$C(x,x') = C(x',x)$$

$$C(x,x') = 0 \text{ if } \|x - x'\| > \delta$$

- **Need nonlocal weak form* $\rightarrow$ Multiply by test function and "integrate by parts"**

$$a(u,v) = -\int_{\overline{\overline{\Omega}}}\int_{\overline{\overline{\Omega}}} C(x,x')\left[u(x') - u(x)\right]v(x)dx'dx$$

$$= \frac{1}{2}\int_{\overline{\overline{\Omega}}}\int_{\overline{\overline{\Omega}}} C(x,x')\left[u(x') - u(x)\right]\left[v(x') - v(x)\right]dx'dx$$

- **Compare with local Poisson operator**
  - **Hooke's law**

$$-\nabla^2 u(x) \quad \Rightarrow \quad \frac{1}{2}\int \nabla u \cdot \nabla v \, dx$$

*E. Emmrich and O. Weckner, *The peridynamic equation and its spatial discretization, Math. Model. Anal.*, 12(1), pp. 17-27, 2007.

Nonlocal Quadrature

- **Local Quadrature (Review)**
  - **One integral required**
  - **Compute products of *gradients* of shape functions and apply Gauss quadrature**
  - **Gradient *drops* polynomial order (lower order quadrature scheme required)**

$$a(u,v) = \frac{1}{2}\int \nabla u \cdot \nabla v \, dx$$

- **Nonlocal Quadrature**
  - ***Two* integrals required**
  - **Compute products of differences of shape functions and integrate**
  - **No gradient $\rightarrow$ higher polynomial order (higher order quadrature needed)**
  - **Nonlocality generates substantially more work over each element**
  - **Discontinuous integrands a challenge for quadrature routines (more later…)**

$$a(u,v) = -\int_{\bar{\bar{\Omega}}}\int_{\bar{\bar{\Omega}}} C(x,x')\left[u(x') - u(x)\right] v(x) dx' dx$$

$$= \frac{1}{2}\int_{\bar{\bar{\Omega}}}\int_{\bar{\bar{\Omega}}} C(x,x')\left[u(x') - u(x)\right]\left[v(x') - v(x)\right] dx' dx$$

- **Integration by parts is standard in local (classical) FEM.**
- **Unclear if there is any computational value in nonlocal setting**

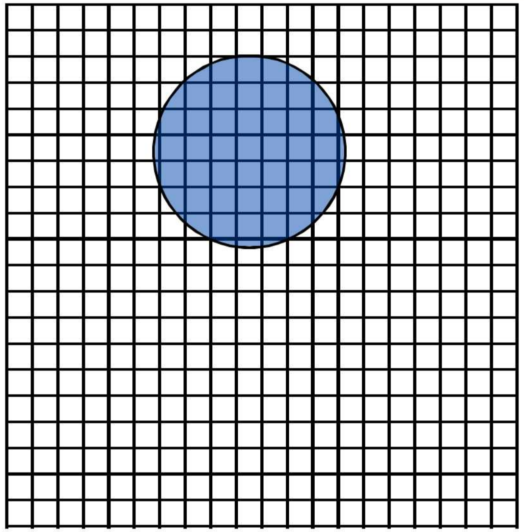
Nonlocal Weak Form – 2D

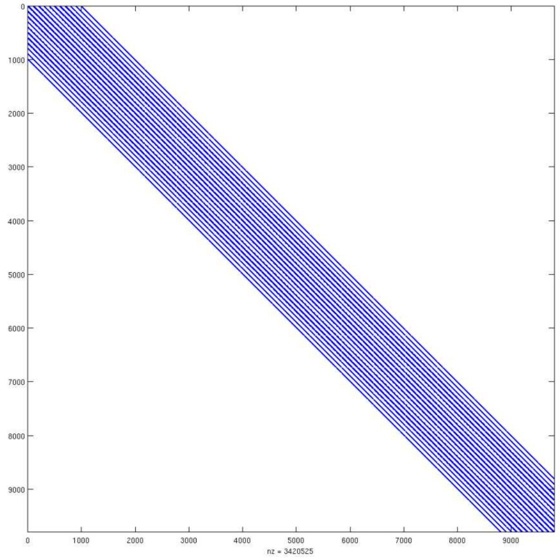
- Let $\Omega = (0,1)\times(0,1)$; u=0 on B$\Omega$

- Weak form requires quadruple integral
  - Expensive!
- Matrix bandwidth controlled by δ/h
  - $\delta \sim |\Omega|$ gives dense matrix (intractable at large scales)
  - Classical FEM has (roughly) constant nnz per row

- Integrand discontinuous!
  - Gauss quadrature not accurate
  - Adaptive quadrature (expensive)
  - Use 1-norm, not 2-norm distance? (blue circle becomes blue square)
  - Break up integral into many separate integrals where integrand continuous over each subregion

- Exact analytic for approach for quadrature?
  - Intractable (so far)
- More practical approach: approximate blue region by simpler geometric shape and then performing quadrature



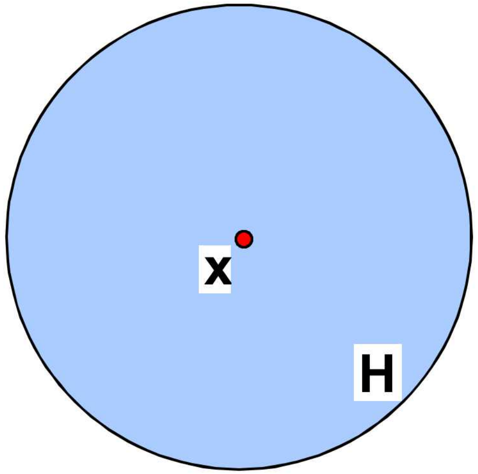


Stiffness Matrix Sparsity Pattern
(10,000 unknowns, 3.4M nnz)

Strong Form Discretization

- **Spatial Discretization**
  - **Approximate integral with sum***
  - **Midpoint quadrature**
  - **Piecewise constant approximation (could go higher)**

Continuum



$$\int_H f(u(x',t) - u(x,t), x' - x)\,dV'$$

*S.A. Silling and E. Askari, *A meshfree method based on the peridynamic model of solid mechanics,* Computers and Structures, 83, pp. 1526-1535, 2005.

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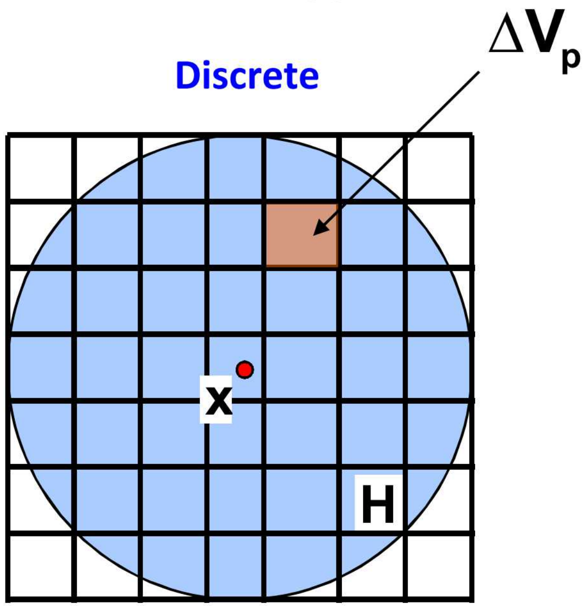

$$\sum_{p} \mathbf{f}(\mathbf{u}(\mathbf{x}_p, t) - \mathbf{u}(\mathbf{x}_i, t), \mathbf{x}_p - \mathbf{x}_i)\Delta V_p$$

*S.A. Silling and E. Askari, *A meshfree method based on the peridynamic model of solid mechanics,* Computers and Structures, 83, pp. 1526-1535, 2005.

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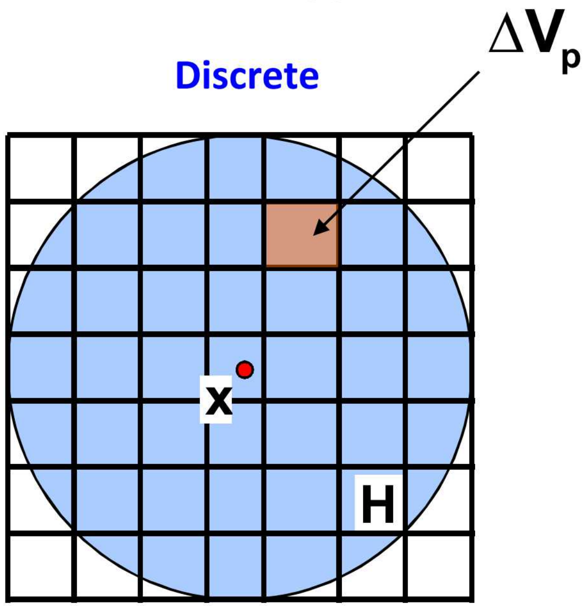


$$\sum_p f(u(x_p,t)-u(x_i,t), x_p - x_i)\Delta V_p$$

- **Temporal Discretization**
  - Explicit central difference in time

$$\ddot{u}(x,t) \approx \ddot{u}_i^n = \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2}$$

  - Velocity-Verlet

$$v_i^{n+1/2} = v_i^n + \left(\frac{\Delta t}{2m}\right) f_i^n$$

$$u_i^{n+1} = u_i^n + (\Delta t) v_i^{n+1/2}$$

$$v_i^{n+1} = v_i^{n+1/2} + \left(\frac{\Delta t}{2m}\right) f_i^{n+1}$$

*S.A. Silling and E. Askari, *A meshfree method based on the peridynamic model of solid mechanics*, Computers and Structures, 83, pp. 1526-1535, 2005.

Asymptotically Compatible Discretizations

Model Convergence (δ Convergence)

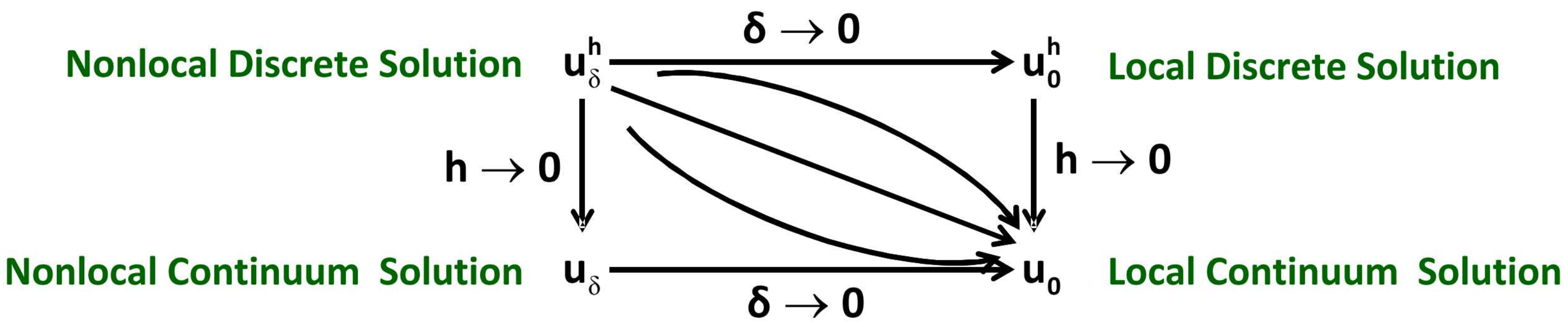
- We are interested in nonlocal models that reduce to their local counterpart as the nonlocal parameter goes to zero.
  - i.e., $\lim_{\delta \to 0} \mathbf{L}_\delta \mathbf{u}_\delta = \mathbf{L}_0 \mathbf{u}_0$
- Example:
  - $\mathbf{L}_\delta \mathbf{u} = \int_{\mathbf{x}-\delta}^{\mathbf{x}+\delta} \mathbf{C}(\mathbf{x},\mathbf{y})(\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x}))d\mathbf{y}, \quad \mathbf{L}_0 \mathbf{u} = \frac{\partial}{\partial \mathbf{x}} \mathbf{k}(\mathbf{x}) \frac{\partial \mathbf{u}}{\partial \mathbf{x}}$
- In general, this must be proven for each specific model or class of models (diffusion, elasticity, plasticity, etc.)
- A simple observation:
  - Let $\mathbf{C}(\mathbf{x},\mathbf{y}) = \frac{3}{\delta^3}\left(\frac{\mathbf{k}(\mathbf{x}) + \mathbf{k}(\mathbf{y})}{2}\right)$
  - Assume we can series expand u(y), k(y) about x. Then,

$$\mathbf{L}_\delta \mathbf{u} = \frac{\partial}{\partial \mathbf{x}} \mathbf{k}(\mathbf{x}) \frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \delta^2 \left(\frac{3}{20} \frac{\partial^2 \mathbf{k}}{\partial^2 \mathbf{x}} \frac{\partial^2 \mathbf{u}}{\partial^2 \mathbf{x}} + \frac{1}{10} \frac{\partial \mathbf{k}}{\partial \mathbf{x}} \frac{\partial^3 \mathbf{u}}{\partial^3 \mathbf{x}} + \dots \right.$$

  - Leading order terms are the local model; all others vanish with δ.
- **Nonlocal models naturally encapsulate many length scales.**

Solution Convergence

- We also desire mesh-convergent solutions.
  - i.e., $\lim_{h \to 0} \mathbf{u}_\delta^h = \mathbf{u}_\delta$
- Thus, it should follow naturally that $\lim_{h,\delta \to 0} \mathbf{u}_\delta^h = \mathbf{u}_0$.
- **It was shown by Q. Du & X. Tian*, ** that this is not always the case!**
  - **The interplay between the length scales h, δ is important!**
- Du & Tian define a general framework for these convergence results**



- **Practical (non-intuitive?) result:**
  - **Piecewise constant discretization converges only if h→0 faster than $\delta \to 0$.**
  - PWC is most common PD discretization; δ **=** κ**h** a common assumption!
  - PWL is asymptotically compatible (i.e., convergent for any sequence h, $\delta \to 0$)

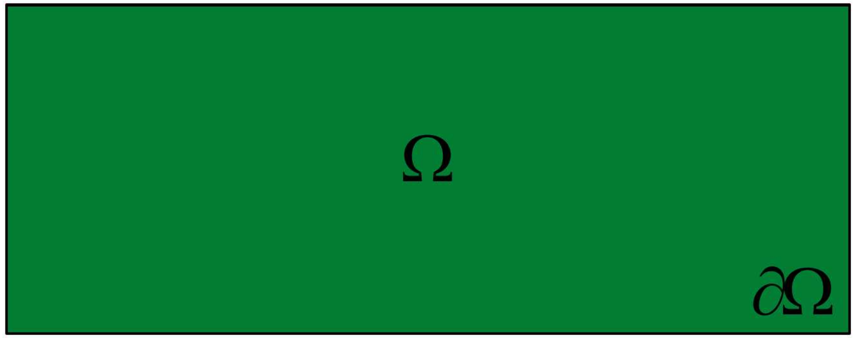
*X. Tian and Q. Du, *Analyis and Comparison of Different Approximations to Nonlocal Diffusion and Linear Peridynamic Equations,* SIAM J. Numer. Anal. , v51(6), pp. 3458–3482, 2013.

** X. Tian and Q. Du, *Asymptotically Compatible Schemes and Applications to Robust Disctretization of Nonlocal Models,* SIAM J. Numer. Anal. , v52(4), pp. 1641–1665, 2014.

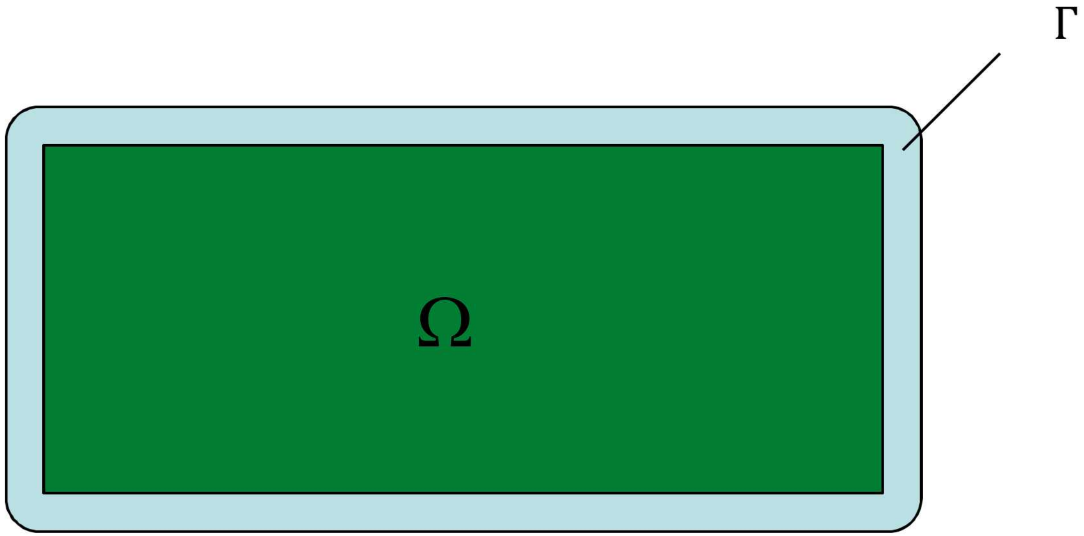
Nonlocal Calculus

Nonlocal Boundaries

- For local models (for example, PDE-based models), we apply boundary conditions on the boundary of the domain (hence the name)



- A Peridynamic "boundary" becomes a volumetric region, sometimes called a "nonlocal boundary", "collar", etc.
- Boundary conditions for these models are called "nonlocal boundary conditions", "volume constraints", etc.



Nonlocal Operators*

❑ Nonlocal Point Divergence

Given a vector two-point function $\mathbf{v}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$ and a symmetric vector-valued function $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$, the nonlocal point divergence operator is a mapping ƛ$_{\alpha}\colon \mathbf{v} \mapsto$ ƛ$_{\alpha}[\mathbf{v}]$, where ƛ$_{\alpha}[\mathbf{v}]\colon \mathbb{R}^n \to \mathbb{R}$ is given by

$$D_{\boldsymbol{\alpha}}[\mathbf{v}](\mathbf{x}) = \int_{\Omega\cup\Gamma} (\mathbf{v}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) - \mathbf{v}(\mathbf{y},\mathbf{x})\cdot\boldsymbol{\alpha}(\mathbf{y},\mathbf{x}))d\mathbf{y} \quad \text{for } \mathbf{x}\in\Omega.$$

❑ Nonlocal Two-Point Gradient

Given a function $u(\mathbf{x})\colon \mathbb{R}^n \to \mathbb{R}$, the formal adjoint of ƛ$_{\alpha}$ is the nonlocal two-point gradient operator □$_{\alpha}\colon u \mapsto$ □$_{\alpha}[u]$, where □$_{\alpha}[u]\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$ is given by

$$G_{\boldsymbol{\alpha}}[u](\mathbf{x},\mathbf{y}) = (u(\mathbf{y}) - u(\mathbf{x}))\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) \quad \text{for} \quad (\mathbf{x},\mathbf{y}) \in \square^n \times \square^n$$

❑ Nonlocal Normal

Given a vector two-point function $\mathbf{v}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$ and a symmetric vector-valued function $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$, the nonlocal normal is a mapping .·˙$_{\alpha}\colon \mathbf{v} \mapsto$.·˙$_{\alpha}[\mathbf{v}]$ where .·˙$_{\alpha}[\mathbf{v}]\colon \mathbb{R}^n \to \mathbb{R}$ is given by

$$N_{\boldsymbol{\alpha}}[u](\mathbf{x}) := -\int_{\Omega\cup\Gamma} (\mathbf{v}(\mathbf{x},\mathbf{y})\cdot\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) - \mathbf{v}(\mathbf{y},\mathbf{x})\cdot\boldsymbol{\alpha}(\mathbf{y},\mathbf{x}))d\mathbf{y} \quad \text{for } \mathbf{x}\in\Gamma$$

* There is also a nonlocal curl; I won't talk about it today.

Familiar Relationships

Nonlocal Gauss Theorem

Given a vector two-point function $\boldsymbol{\nu}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$, we have

$$\int_\Omega \mathrm{D}_{\boldsymbol{\alpha}}[\boldsymbol{\nu}](\mathbf{x})d\mathbf{x} = \int_\Gamma \mathrm{N}_{\boldsymbol{\alpha}}[\boldsymbol{\nu}](\mathbf{x})d\mathbf{x}$$

Nonlocal Integration by Parts

Given a function $\mathrm{u}(\mathbf{x})\colon \mathbb{R}^{\mathbf{n}} \to \mathbb{R}$, $\boldsymbol{\nu}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$, and a symmetric vector-valued function $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$, we have

$$\int_\Omega \mathrm{u}(\mathbf{x})\mathrm{D}_{\boldsymbol{\alpha}}[\boldsymbol{\nu}](\mathbf{x})d\mathbf{x} - \int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \mathrm{G}_{\boldsymbol{\alpha}}[\mathrm{u}](\mathbf{x},\mathbf{y})\cdot\nu(\mathbf{x},\mathbf{y})d\mathbf{y}d\mathbf{x} = \int_\Gamma \mathrm{u}(\mathbf{x})\mathrm{N}_{\boldsymbol{\alpha}}[\boldsymbol{\nu}](\mathbf{x})d\mathbf{x}$$

Nonlocal Green's First Identity

Given the function $\mathrm{u}(\mathbf{x}), \mathrm{v}(\mathbf{x})\colon \mathbb{R}^{\mathbf{n}} \to \mathbb{R}$, and a symmetric vector-valued function $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^k$, we have

$$\int_\Omega \mathrm{u}(\mathbf{x})\mathrm{D}_{\boldsymbol{\alpha}}\left[\mathrm{G}_{\boldsymbol{\alpha}}[\mathrm{v}]\right](\mathbf{x})d\mathbf{x} - \int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \mathrm{G}_{\boldsymbol{\alpha}}[\mathrm{u}](\mathbf{x},\mathbf{y})\cdot\mathrm{G}_{\boldsymbol{\alpha}}[\mathrm{v}](\mathbf{x},\mathbf{y})d\mathbf{y}d\mathbf{x} = \int_\Gamma \mathrm{u}(\mathbf{x})\mathrm{N}_{\boldsymbol{\alpha}}[\mathrm{G}_{\boldsymbol{\alpha}}[\mathrm{v}]](\mathbf{x})d\mathbf{x}$$

Nonlocal Laplacian

We can compose nonlocal operators in familiar ways.

❑ Nonlocal Laplacian

Given a function $\mathbf{u}(\mathbf{x})\colon \mathbb{R}^{\mathbf{n}} \to \mathbb{R}$ and $\boldsymbol{\mu}(\mathbf{x},\mathbf{y}) = \boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})$ where $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\colon \mathbb{R}^{\mathbf{n}} \times \mathbb{R}^{\mathbf{n}} \to \mathbb{R}^{\mathbf{k}}$ is a symmetric vector-valued function, the nonlocal Laplace operator is defined as

$$\mathrm{L}_{\mu}[\mathrm{u}](\mathbf{x}) := \mathrm{D}_{\boldsymbol{\alpha}}\left[\mathrm{G}_{\boldsymbol{\alpha}}[\mathrm{u}]\right](\mathbf{x}) = 2\int_{\Omega\cup\Gamma} (\mathrm{u}(\mathbf{y}) - \mathrm{u}(\mathbf{x}))\mu(\mathbf{x},\mathbf{y})d\mathbf{y} \quad \text{for} \quad \mathbf{x} \in \Omega$$

❑ Nonlocal Poisson Equation (Dirichlet Boundary Conditions)

$$\begin{aligned} \mathrm{L}_{\mu}[\mathrm{u}](\mathbf{x}) &= \mathrm{b}(\mathbf{x}) \quad \text{for} \quad \mathbf{x} \in \Omega \\ \mathrm{u}(\mathbf{x}) &= \mathrm{g}(\mathbf{x}) \quad \text{for} \quad \mathbf{x} \in \Gamma \end{aligned}$$

Conditioning Results

Background: Condition Number

We denote the condition number of A as $\kappa(A) := \|A\|\|A^{-1}\|$.

We can demonstrate its usefulness via perturbation analysis. Let Ax=b and consider the perturbed system:

- $(A + \varepsilon E)x(\varepsilon) = b + \varepsilon e$

Let $\delta(\varepsilon) = x(\varepsilon) - x$. Then,

- $(A + \varepsilon E)\delta(\varepsilon) = b + \varepsilon e - (b - \varepsilon E)$
- $(A + \varepsilon E)\delta(\varepsilon) = \varepsilon(e - Ex)$
- $\delta(\varepsilon) = \varepsilon(A + \varepsilon E)^{-1}(e - Ex)$

We observe that the function $x(\varepsilon)$ is differentiable at ε=0:

- $x'(0) = \lim_{\varepsilon \to 0} \frac{x(0+\varepsilon) - x(0)}{\varepsilon} = A^{-1}(e - Ex)$

Perturbing the pair (A,b) by the small amount (εE,εe) will cause the solution to change by $\varepsilon x'(0)$. Thus,

- $\|x(\varepsilon) - x\| = \varepsilon\|A^{-1}(e - Ex)\|$
- $\|x(\varepsilon) - x\| \le \varepsilon\|A^{-1}\|(\|e\| + \|E\|\|x\|) + O(\varepsilon^2)$

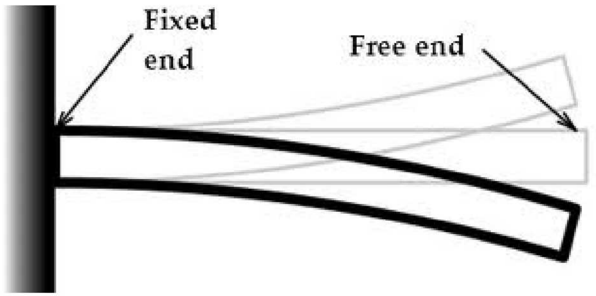
Further simplification and use of the relationship $\|b\| \le \|A\|\|x\|$ gives the relative variation in the solution to the relative sizes of the perturbation

- $\frac{\|x(\varepsilon) - x\|}{\|x\|} \le \varepsilon\|A^{-1}\|\|A\|\left(\frac{\|e\|}{\|b\|} + \frac{\|E\|}{\|A\|}\right) + O(\varepsilon^2)$

Background: Condition Number

What does this mean physically?

- For Ill-conditioned systems, small perturbation in input can result in a large change in solution

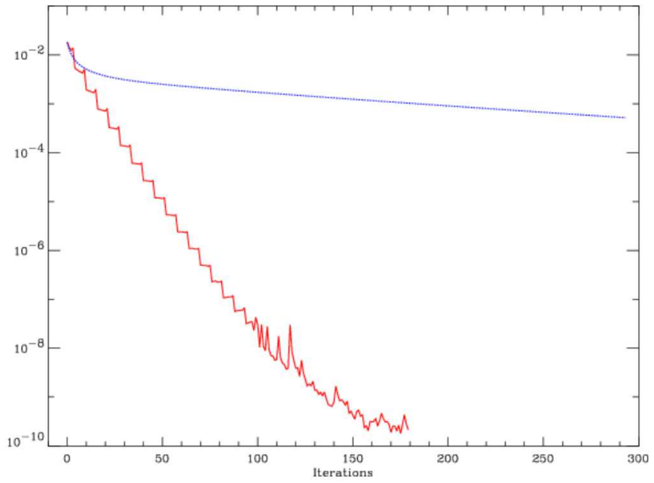


Cantilevered beam

What does this mean for linear solvers?

- Condition number dictates accuracy
  - Using relationships Ax=b, e=A^{-1}r, can show that $\frac{\|e\|}{\|x\|} \leq \|A\|\|A^{-1}\| \frac{\|r\|}{\|b\|}$
  - Small relative residual does not imply small relative error!

- Condition number dictates convergence rate
  - Convergence rate of conjugate gradients: $\|e^{(k)}\|_A \leq 2 \left(\frac{\sqrt{\kappa(A)}-1}{\sqrt{\kappa(A)}+1}\right)^k \|e^{(0)}\|_A$



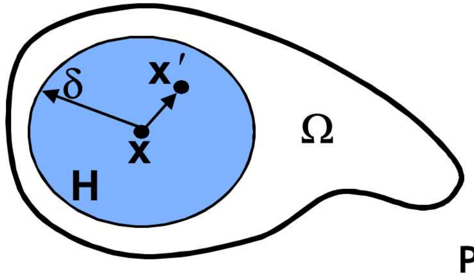
Convergence curves for optimal Krylov methods

Conditioning of Peridynamic Operators

- **Why is conditioning important?**
  - Condition number dictate convergence rates of linear solvers
  - Condition numbers dictate the accuracy of computed solution
  - Rule of thumb:

    If $\kappa(A) = 10^{16-d}$, then computed solution has d digits of accuracy (double precision)

    If $\kappa(A) = 10^{16}$, expect zero digits of accuracy!
- Old saying: ***"You get the answer you deserve…"***



Point x interacts directly with all points x' within H

- **New component in nonlocal modeling is peridynamic horizon δ**
  - How does δ affect the conditioning?
  - Develop preconditioners/solvers optimized for nonlocal models at extreme scales

- To explore the effects of conditioning, let's consider a FEM discretization of peridynamics

*E. Emmrich and O. Weckner, *The peridynamic equation and its spatial discretization, Math. Model. Anal.,* 12(1), pp. 17-27, 2007.

Spectral Equivalence

- For simplicity, assume

$$C(x,x') = \chi_\delta(x - x') \equiv \begin{cases} 1 & \text{if } \|x - x'\| \le \delta \\ 0 & \text{otherwise} \end{cases}$$

"Canonical" Kernel Function

- Main Theorem*

$$\lambda_1(\bar{\bar{\Omega}})\delta^{d+2} \le \frac{a(u,u)}{\|u\|_{L_2(\bar{\bar{\Omega}})}} \le \lambda_2(\bar{\bar{\Omega}})\delta^{d} \qquad u \in L_{2,0}(\bar{\bar{\Omega}})$$

- Let K be a finite element discretization of a(u,u). Then, in h << δ limit,

$$\kappa(K) \sim \mathcal{O}(\delta^{-2})$$

- Dominant length scale in nonlocal model set by δ.
  - Contrast with local model, where length scaled introduced by h
  - **Mesh-independent condition number bound!**

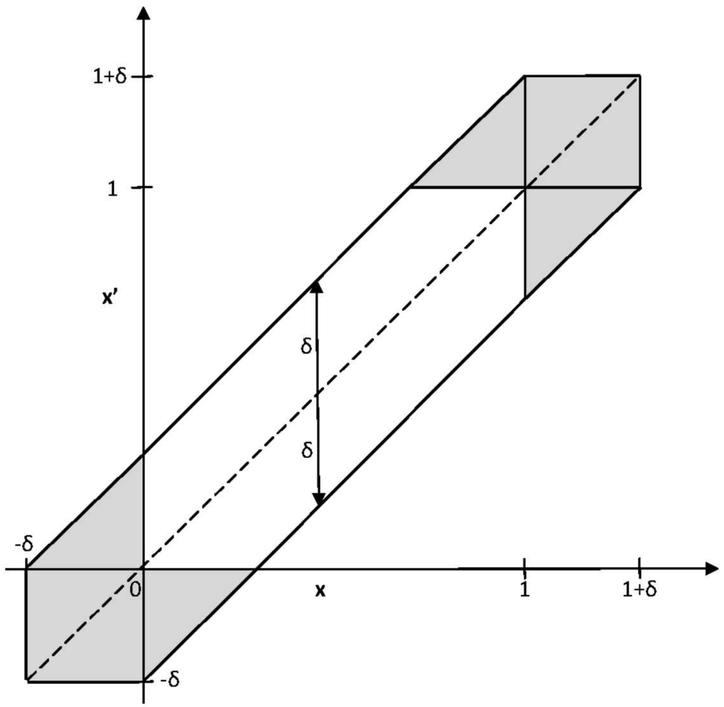
*B. Aksoylu and M.L. Parks, Variational Theory and Domain Decomposition for Nonlocal Problems. Applied Mathematics and Computation, 217, pp. 6498-6515, 2011.

Conditioning Results – 1D

- Let $\Omega = (0,1)$, $\mathcal{B}\Omega = [-\delta,0] \cup [1, \delta]$.
- $u=0$ on $\mathcal{B}\Omega$
- Let $C(x,x') = \begin{cases} 1 & \text{if } \|x - x'\| \le \delta \\ 0 & \text{otherwise} \end{cases}$
- Weak form becomes

$$a(u,v) = -\int_0^1 \int_{x-\delta}^{x+\delta} [u(x') - u(x)]\, v(x)\, dx'\, dx$$

- Numerical Study
  - PW constant and PW linear SFs
  - Hold δ fixed, vary h
  - Hold h fixed, vary δ



Integration Domain in (x,x')
(grey = outside Ω)

*B. Aksoylu and M.L. Parks, Variational Theory and Domain Decomposition for Nonlocal Problems. Applied Mathematics and Computation, 217, pp. 6498-6515, 2011.

Conditioning Results – 1D

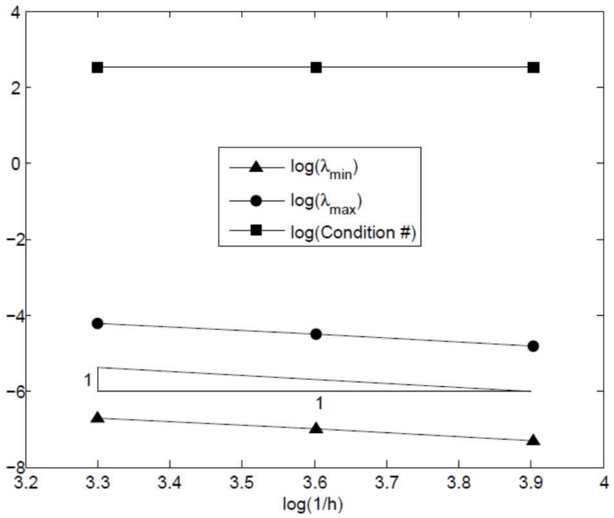
- Observations: $\kappa(K)$~$O(\delta^{-2})$, only weak h-dependence

(a) Constant δ, vary h.

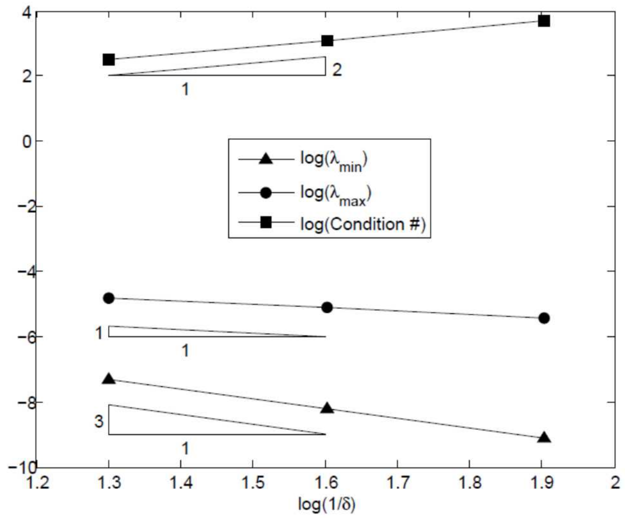
		Piecewise Constant Shape Functions			Piecewise Linear Shape Functions		
$1/h$	$1/\delta$	λ_{min}	λ_{max}	Condition #	λ_{min}	λ_{max}	Condition #
2000	20	1.94E-07	6.07E-05	3.13E+02	1.94E-07	6.07E-05	3.13E+02
4000	20	9.69E-08	3.04E-05	3.13E+02	9.69E-08	3.04E-05	3.14E+02
8000	20	4.84E-08	1.52E-05	3.14E+02	4.84E-08	1.52E-05	3.14E+02

(b) Constant h, vary δ.

		Piecewise Constant Shape Functions			Piecewise Linear Shape Functions		
$1/h$	$1/\delta$	λ_{min}	λ_{max}	Condition #	λ_{min}	λ_{max}	Condition #
8000	20	4.84E-08	1.52E-05	3.15E+02	4.84E-08	1.52E-05	3.14E+02
8000	40	6.24E-09	7.61E-06	1.22E+03	6.24E-09	7.60E-06	1.22E+03
8000	80	7.92E-10	3.80E-06	4.80E+03	7.91E-10	3.80E-06	4.80E+03



(a) Constant δ, vary h.



(b) Constant h, vary δ.

*B. Aksoylu and M.L. Parks, Variational Theory and Domain Decomposition for Nonlocal Problems. Applied Mathematics and Computation, 217, pp. 6498-6515, 2011.

Conditioning Results – 2D

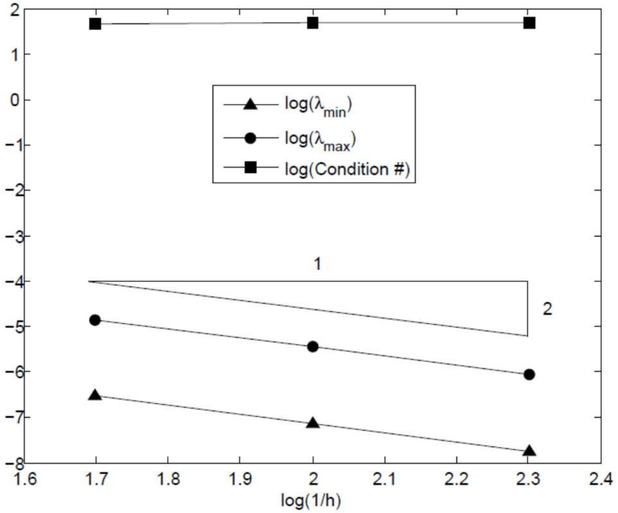
- Do exact quadrature (no quadrature error)
- Observations: $\kappa(K) \sim O(\delta^{-2})$, weak h-dependence

(a) Constant δ, vary h.

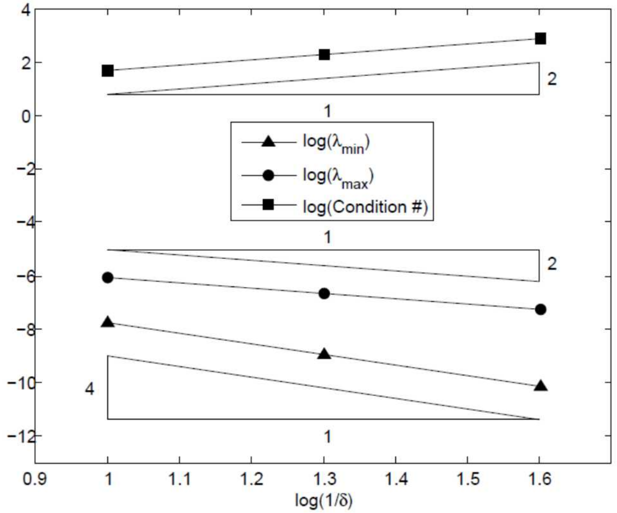
$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
50	10	2.95E-07	1.40E-05	4.77E+01
100	10	7.11E-08	3.54E-06	4.97E+01
200	10	1.75E-08	8.86E-07	5.05E+01

(b) Constant h, vary δ.

$1/h$	$1/\delta$	$\lambda_{\min}$	$\lambda_{\max}$	Condition #
200	10	1.75E-08	8.86E-07	5.05E+01
200	20	1.17E-09	2.22E-07	1.90E+02
200	40	7.63E-11	5.50E-08	7.21E+02



(a) Constant δ, vary h.



(b) Constant h, vary δ.

*B. Aksoylu and M.L. Parks, Variational Theory and Domain Decomposition for Nonlocal Problems. Applied Mathematics and Computation, 217, pp. 6498-6515, 2011.

More General Results

- Consider a more general kernel …

$$a(u,u) = \frac{1-s}{\delta^{2-2s}} \int_{\overline{\Omega}} \int_{H_x} \frac{(u(y)-u(x))^2}{|y-x|^{d+2s}} dydx, \qquad u \in H^s(\overline{\overline{\Omega}}), \quad s \in (0,1)$$

- Can capture h-, δ -, and s-quantification of conditioning (Aksoylu & Unlu, 2015, Zhou & Du, 2010)

$$\kappa(A) \le c \min\left\{ h^{-2s} \delta^{-(2-2s)}, h^{-2} \right\}$$

- Note interplay of δ, h

Summary

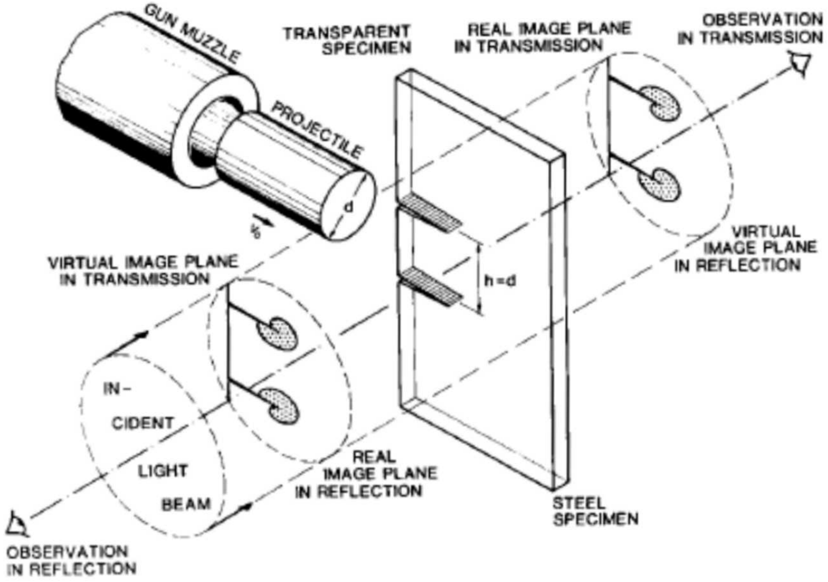
Summary: Survey of Computational Peridynamics

- Local Models, Nonlocal Models, and Length Scales
- Peridynamics overview
- Example computations
- Material models and fracture models
  - Linear isotropic elastic
  - Elastic-plastic
  - Viscoelastic
  - Brittle and ductile failure
- Discretizations and numerical methods
  - Weak form discretization
  - Strong form discretization
- Asymptotically Compatible Discretizations
- Nonlocal Calculus
- Condition Number Analysis

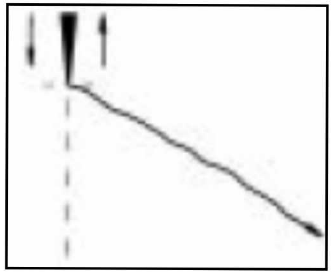
Kalthoff-Winkler Experiment

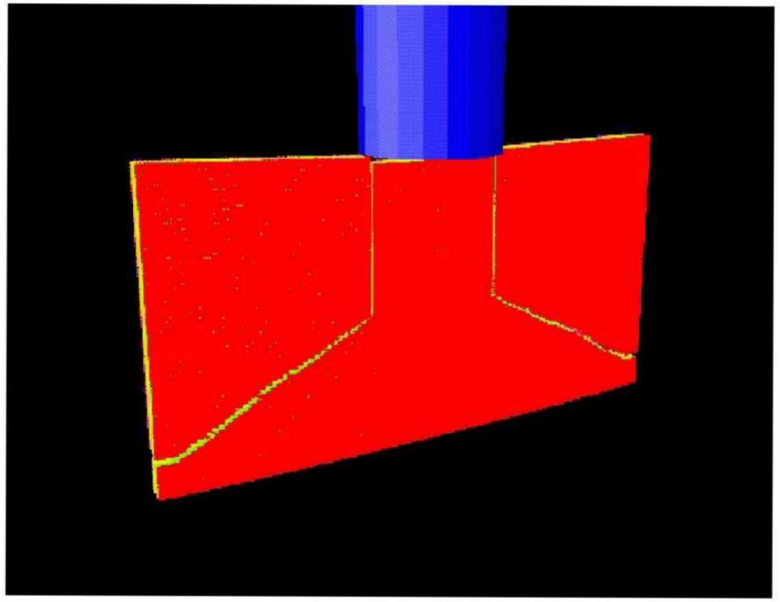
- ❑ **Dynamic fracture in steel (Kalthoff & Winkler, 1988)**
- ❑ **Mode-II loading at notch tips results in mode-I cracks at 70o angle**
- ❑ **Peridynamic model reproduces the crack angle observed experimentally***

Simulation performed with EMU



Experimental Results





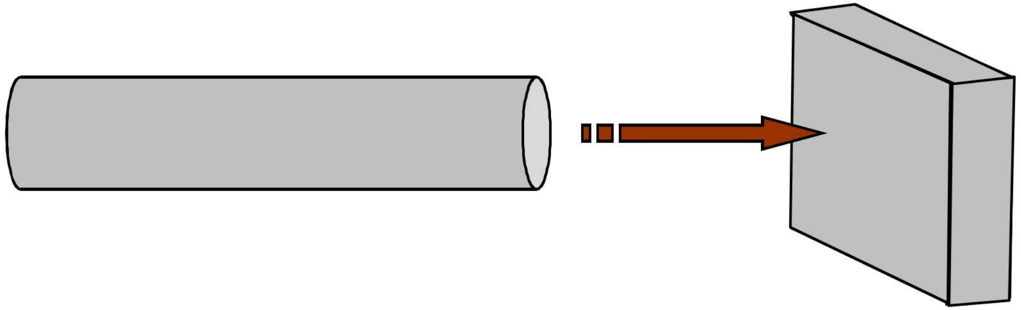
Peridynamic Model

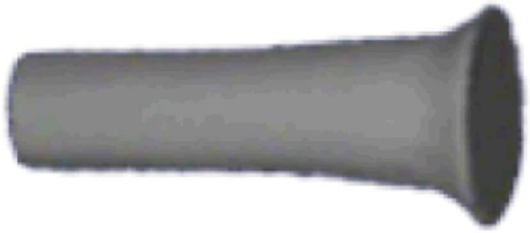
* S. A. Silling, Dynamic fracture modeling with a meshfree peridynamic code, in Computational Fluid and Solid Mechanics 2003, K.J. Bathe, ed., Elsevier, pp. 641-644.

Taylor Bar Test

- ❑ **Taylor impact test of 6061-T6 aluminum***

Simulation performed with EMU





Experiment

Peridynamic Model*

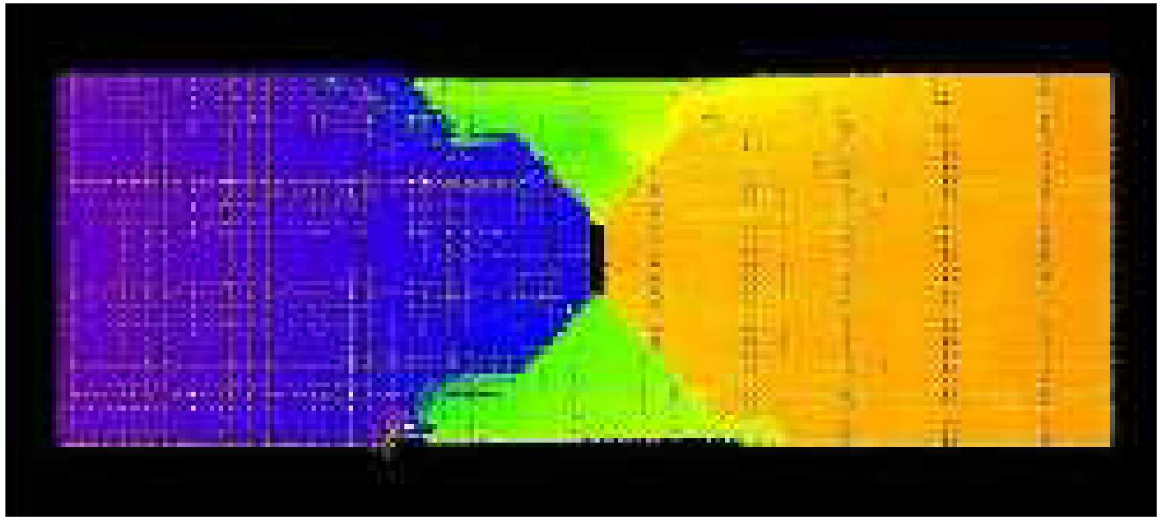
* J. Foster, S.A. Silling, W.W. Chen, Viscoplasticity Using Peridynamics, Sandia National Laboratories Technical Report SAND2008-7835, 2008.

Failure in Fiber-Reinforced Composites

- **Splitting and fracture mode changes in fiber-reinforced composites***
- **Fiber orientation between plies strongly influences crack growth**

Simulation performed with EMU

Typical crack growth in notched laminate (photo courtesy Boeing)



Peridynamic Model

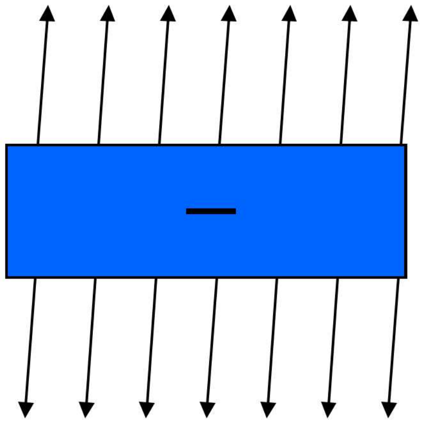
* E. Askari, F. Bobaru, R.B. Lehoucq, M.L. Parks, S.A. Silling, O.Weckner, Peridynamics for multiscale materials modeling, in SciDAC 2008, Seattle, Washington, vol. 125 of Journal of Physics: Conference Series, (012078) 2008.

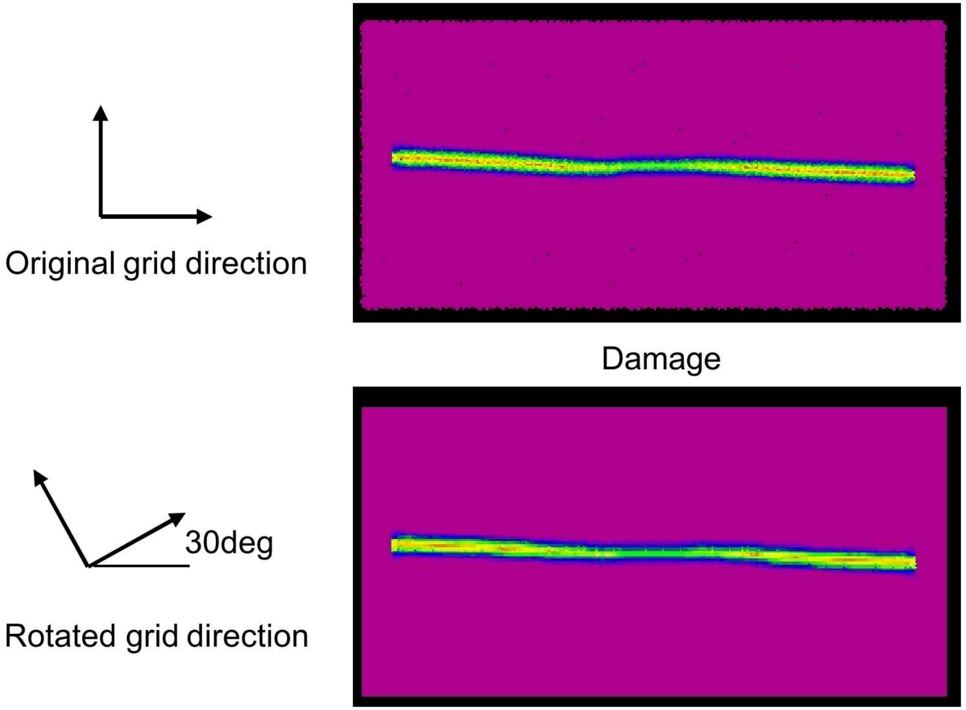
Mesh-Independent Crack Growth

- ❑ **Discrete peridynamic model exhibits mesh-independent crack growth**
- ❑ **Plate with a pre-existing defect is subjected to prescribed boundary velocities**
- ❑ **Crack growth direction depends continuously on loading direction**

Simulation performed with EMU

$$\dot{\varepsilon} = (0.25\mathrm{s}^{-1}) \begin{bmatrix} 0 & 0.1 \\ 0 & 1 \end{bmatrix}$$



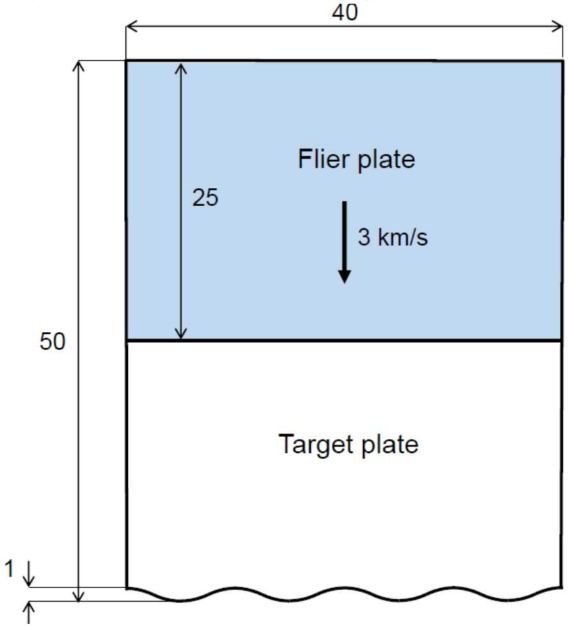


- ❑ **Nonlocal network of bonds in many directions allows cracks to grow in any direction.**

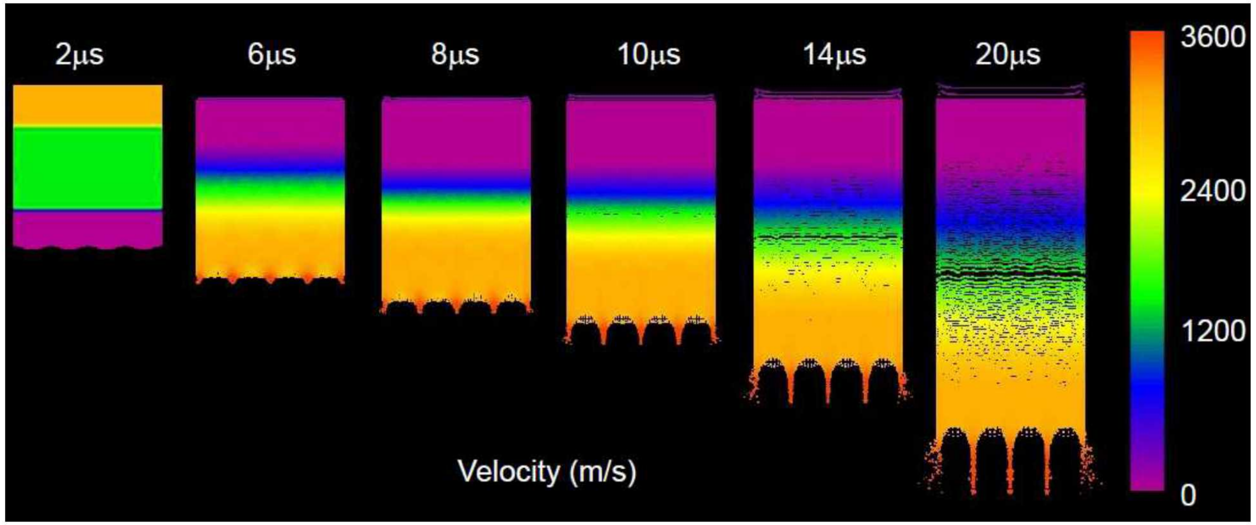
Shockwave Ejecta

- Motivated by experiments by Ogorodnikov et al.*
- Utilize Peridynamic Eulerian model with Mie-Grüneisen EOS
- Impact aluminum flyer plate on aluminum target plate at 3 km/s, pressure 30 Gpa

Simulation performed with EMU



Initial geometry.
Dimensions in mm.



Peridynamic simulation results.
Six different simulation times are shown.

- **Computed shock velocity is 7.140 km/s; Expected value is 7.230 km/s.**
- **Computed jet tip velocity is 4.0 km/s; Experimentally measured value is 3.7 km/s.**

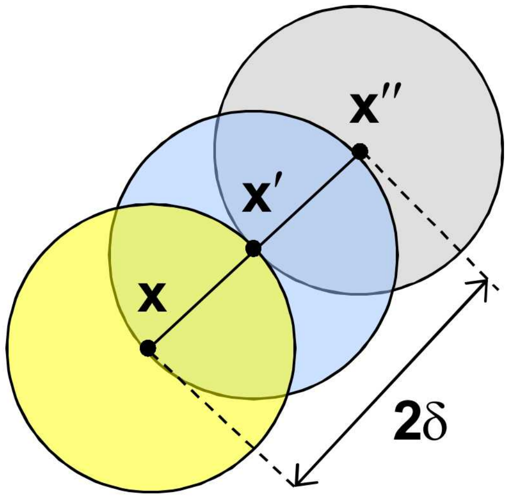
* V. A. Ogorodnikov, A. L. Mikhailov, A. V. Romanov, A. A. Sadovoi, S. S. Sokolov, and O. A. Gorbenko, Modeling jet flows caused by the incidence of a shock wave on a profiled free surface, Journal of Applied Mechanics and Technical Physics, 48 (2007), pp. 11–16.

Maximum Interaction Distance

- **Recall the linear peridynamic solid (LPS) model**

$$\rho\ddot{\mathbf{u}}(\mathbf{x},t)=\int_{H}\left(\mathbf{T}[\mathbf{x},t]\langle\mathbf{x}'-\mathbf{x}\rangle-\mathbf{T}[\mathbf{x}',t]\langle\mathbf{x}-\mathbf{x}'\rangle\right)dV_{\mathbf{x}'}+\mathbf{b}(\mathbf{x},t)$$

$$\mathbf{T}[\mathbf{x},t]\langle\mathbf{x}'-\mathbf{x}\rangle=\left(\frac{3k\theta}{m}\underline{\omega}\underline{\mathbf{x}}+\frac{15\mu}{m}\underline{\omega}\underline{\mathbf{e}}^{d}\right)\frac{\mathbf{x}'-\mathbf{x}}{\|\mathbf{x}'-\mathbf{x}\|}$$



- **The dilatation is defined as** $\theta=\frac{3}{m}\int_{H}\underline{\omega}\underline{\mathbf{x}}\underline{\mathbf{e}}dV$

- **Movement at x'' influences dilatation at x'.**
- **Dilatation at x' influences force state at x.**

- **In the state-based theory, the effective interaction distance is 2δ!**
  - **Affects communication patterns**
  - **Affects stiffness matrix bandwidth (~ 2δ/h, not δ/h)**